



Full wwPDB EM Validation Report ⓘ

Nov 28, 2022 – 09:57 AM EST

PDB ID : 7LS2
EMDB ID : EMD-23501
Title : 80S ribosome from mouse bound to eEF2 (Class I)
Authors : Loerch, S.; Smith, P.R.; Kunder, N.; Stanowick, A.D.; Lou, T.-F.; Campbell, Z.T.
Deposited on : 2021-02-17
Resolution : 3.10 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:

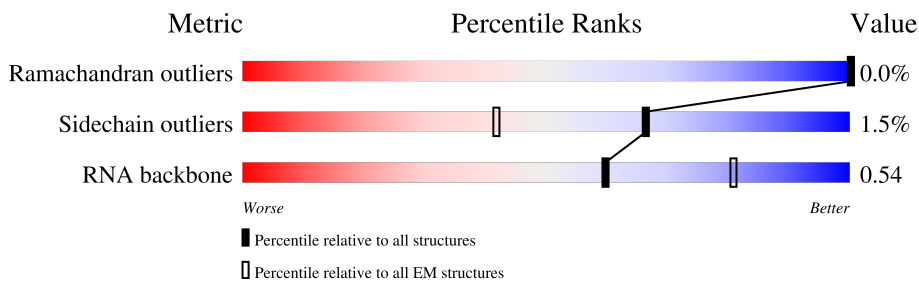
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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	A1	270	
2	B1	266	
3	C1	192	
4	D1	214	
5	E1	178	
6	F1	211	
7	G1	217	
8	H1	204	

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Mol	Chain	Length	Quality of chain
9	A2	4731	60% 17% 22%
10	B2	121	86% 13%
11	C2	156	81% 18%
12	D2	257	96%
13	E2	403	98%
14	F2	419	87% 12%
15	G2	297	99%
16	H2	296	74% 25%
17	I2	203	98%
18	J2	184	83% 17%
19	K2	188	99%
20	L2	196	92% 6%
21	M2	176	99%
22	N2	160	98%
23	O2	128	79% 21%
24	P2	140	91% 8%
25	Q2	157	8% 69% 30%
26	R2	156	76% 24%
27	S2	145	90% 8%
28	T2	136	99%
29	U2	148	99%
30	V2	160	8% 71% 27%
31	W2	115	81% 18%
32	X2	125	85% 14%
33	Y2	135	94% 5%

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Mol	Chain	Length	Quality of chain
34	Z2	110	97%
35	a2	117	96%
36	b2	123	98%
37	c2	105	96%
38	d2	97	88% 11%
39	e2	70	99%
40	f2	51	98%
41	g2	128	40% 59%
42	h2	25	96%
43	i2	106	92% 5%
44	j2	92	95%
45	k2	137	90% 9%
46	m2	1871	71% 21% 8%
47	n2	75	5% 68% 32%
48	p2	264	81% 19%
49	q2	243	92% 7%
50	r2	263	98%
51	w2	158	9% 95%
52	z2	135	98%
53	o2	295	73% 27%
54	s2	204	10% 92% 7%
55	v2	165	58% 41%
56	x2	145	87% 10%
57	y2	146	98%
58	A3	152	93% 5%

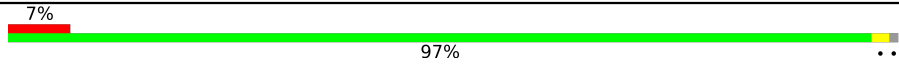
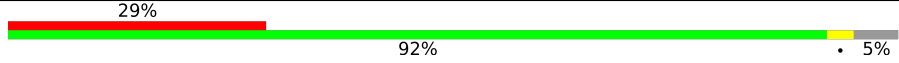
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Mol	Chain	Length	Quality of chain
59	B3	145	95%
60	C3	119	85% 14%
61	D3	83	100%
62	E3	143	98%
63	F3	115	83% 13%
64	G3	69	93% 7% 16%
65	H3	56	95%
66	I3	317	96%
67	J3	293	75% 24%
68	K3	249	90% 9%
69	L3	194	93% 5%
70	M3	132	92% 8% 27%
71	N3	151	99%
72	O3	151	87% 11%
73	P3	130	98%
74	Q3	133	97% 7%
75	R3	125	60% 40%
76	S3	84	96%
77	T3	133	41% 59%
78	U3	156	37% 60%
79	m	858	97%
80	j	317	61% 38%
81	k	165	90% 7%
82	A	386	84%
83	t	194	92% 6%

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Mol	Chain	Length	Quality of chain
84	u	208	 <p>7% 97% ..</p>
85	L1	217	 <p>29% 92% 5%</p>

2 Entry composition [i](#)

There are 89 unique types of molecules in this entry. The entry contains 227130 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 protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A1	222	1851	1190	356	297	8	1	0

- Molecule 2 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B1	230	1863	1188	359	312	4	1	0

- Molecule 3 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C1	190	1519	956	284	273	6	0	0

- Molecule 4 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D1	208	1690	1073	327	278	12	0	0

- Molecule 5 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E1	174	1397	880	260	251	6	0	0

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F1	207	1676	1048	344	280	4	0	0

- Molecule 7 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G1	139	1143	732	221	183	7	0	0

- Molecule 8 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H1	203	1701	1072	359	266	4	0	0

- Molecule 9 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	A2	3706	79519	35463	14497	25854	3705	0	0

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	B2	120	2558	1141	456	842	119	0	0

- Molecule 11 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	C2	156	3315	1481	585	1094	155	0	0

- Molecule 12 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D2	251	1921	1204	393	318	6	0	0

- Molecule 13 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E2	402	3238	2060	609	555	14	0	0

- Molecule 14 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F2	367	2928	1842	583	488	15	0	0

- Molecule 15 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G2	293	2385	1506	440	425	14	0	0

- Molecule 16 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H2	221	1789	1145	342	298	4	0	0

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I2	201	1640	1055	320	259	6	0	0

- Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	J2	153	1242	777	241	215	9	0	0

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	K2	186	1511	946	313	248	4	0	0

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L2	184	1542	955	332	246	9	0	0

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M2	175	1450	924	283	233	10	0	0

- Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	N2	159	1298	823	253	216	6	0	0

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	O2	101	825	529	144	150	2	0	0

- Molecule 24 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	P2	129	969	613	182	169	5	0	0

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q2	110	895	563	180	148	4	0	0

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R2	118	967	618	181	167	1	0	0

- Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	S2	134	1115	700	226	186	3	0	0

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T2	135	1107	714	208	182	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	U2	147	1164	736	239	185	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	V2	117	945	596	198	146	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	W2	94	732	465	130	131	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	X2	107	888	560	171	155	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Y2	128	1053	667	216	165	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Z2	109	876	555	174	143	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a2	114	Total	C	N	O	S	0	0
			906	565	187	148	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b2	120	Total	C	N	O	S	0	0
			1001	634	201	165	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c2	102	Total	C	N	O	S	0	0
			827	516	173	133	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d2	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e2	69	Total	C	N	O	S	0	0
			568	365	103	99	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f2	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g2	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h2	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i2	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j2	89	Total	C	N	O	S	0	0
			694	436	133	118	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k2	125	Total	C	N	O	S	0	0
			1001	621	207	168	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m2	1724	Total	C	N	O	P	0	0
			36817	16440	6606	12048	1723		

- Molecule 47 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n2	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p2	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q2	226	Total	C	N	O	S	0	0
			1756	1119	316	314	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r2	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 51 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w2	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 52 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z2	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	o2	214	Total	C	N	O	S	0	0
			1694	1077	297	312	8		

- Molecule 54 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	s2	189	Total	C	N	O	S	0	0
			1496	934	285	270	7		

- Molecule 55 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v2	97	Total	C	N	O	S	0	0
			819	534	147	133	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	x2	130	1073	681	205	180	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	y2	144	1143	726	216	198	3	0	0

- Molecule 58 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	A3	144	1190	746	241	202	1	0	0

- Molecule 59 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	B3	141	1104	691	215	196	2	0	0

- Molecule 60 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	C3	102	807	507	153	143	4	0	0

- Molecule 61 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	D3	83	638	392	119	122	5	0	0

- Molecule 62 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	E3	141	1098	693	219	183	3	0	0

- Molecule 63 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	F3	100	Total	C	N	O	S	1	0
			811	506	169	131	5		

- Molecule 64 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	G3	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 65 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	H3	54	Total	C	N	O	S	0	0
			455	284	93	73	5		

- Molecule 66 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	I3	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 67 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	J3	222	Total	C	N	O	S	0	0
			1725	1116	298	302	9		

- Molecule 68 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	K3	227	Total	C	N	O	S	0	0
			1840	1149	367	317	7		

- Molecule 69 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	L3	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 70 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	M3	122	Total	C	N	O	S	0	0
			942	593	164	177	8		

- Molecule 71 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	N3	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 72 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	O3	134	Total	C	N	O	S	0	0
			1002	612	197	187	6		

- Molecule 73 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	P3	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 74 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Q3	129	Total	C	N	O	S	0	0
			1049	662	206	176	5		

- Molecule 75 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	R3	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 76 is a protein called 40S ribosomal protein S27-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	S3	83	Total	C	N	O	S	0	0
			652	409	121	115	7		

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	T3	55	Total	C	N	O	S	0	0
			438	271	95	71	1		

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	U3	62	Total	C	N	O	S	0	0
			505	317	96	85	7		

- Molecule 79 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	m	851	Total	C	N	O	S	0	0
			6649	4217	1146	1242	44		

- Molecule 80 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	j	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 81 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	k	153	Total	C	N	O	S	0	0
			1159	721	218	217	3		

- Molecule 82 is a protein called Isoform 3 of Plasminogen activator inhibitor 1 RNA-binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	A	61	Total	C	N	O	0	0
			486	289	94	103		

- Molecule 83 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	t	183	Total	C	N	O	S	0	0
			1477	944	270	262	1		

- Molecule 84 is a protein called 40S ribosomal protein S8.

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

- Molecule 85 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	L1	206	1660	1061	300	291	8	0	0

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	d2	1	Total 1	Zn 1	0
86	g2	1	Total 1	Zn 1	0
86	i2	1	Total 1	Zn 1	0
86	j2	1	Total 1	Zn 1	0
86	F3	1	Total 1	Zn 1	0
86	H3	1	Total 1	Zn 1	0
86	U3	1	Total 1	Zn 1	0

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	H3	1	Total 1	Mg 1	0

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
88	m	1	28	10	5	11	2	0

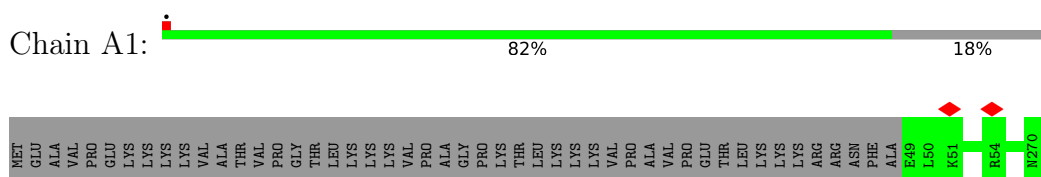
- Molecule 89 is water.

Mol	Chain	Residues	Atoms		AltConf
89	B1	1	Total	O	0
			1	1	
89	A2	1	Total	O	0
			1	1	
89	m2	2	Total	O	0
			2	2	

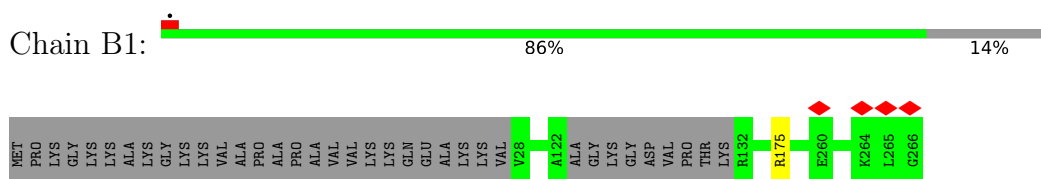
3 Residue-property plots [i](#)

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

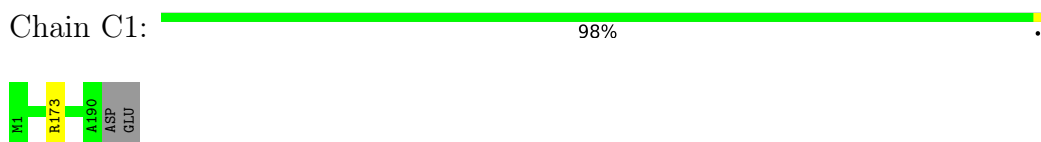
- Molecule 1: 60S ribosomal protein L7



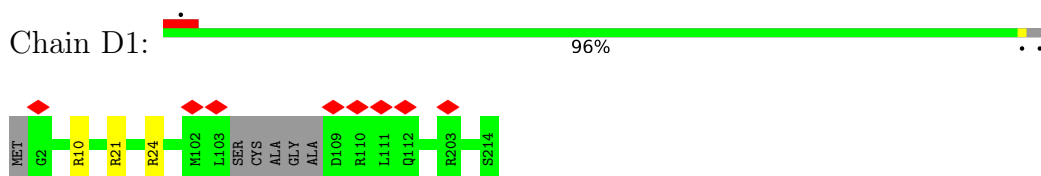
- Molecule 2: 60S ribosomal protein L7a



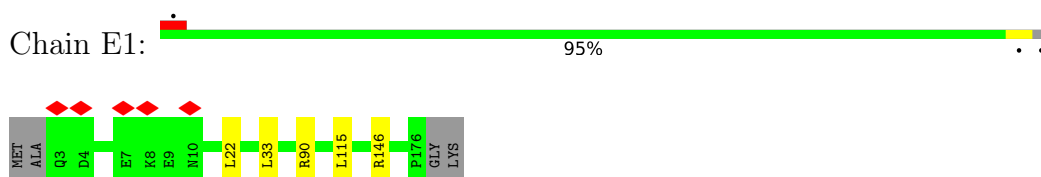
- Molecule 3: 60S ribosomal protein L9

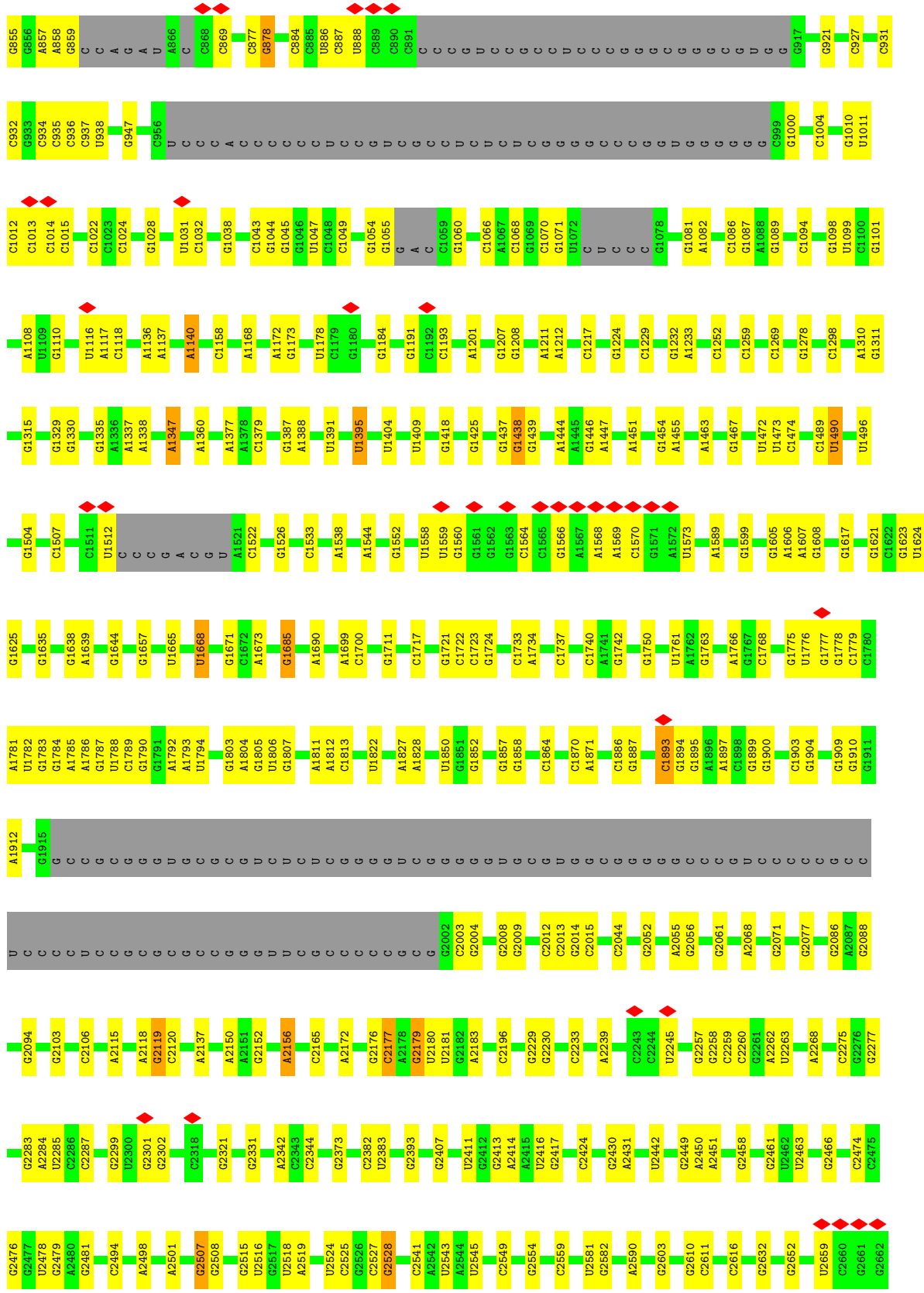


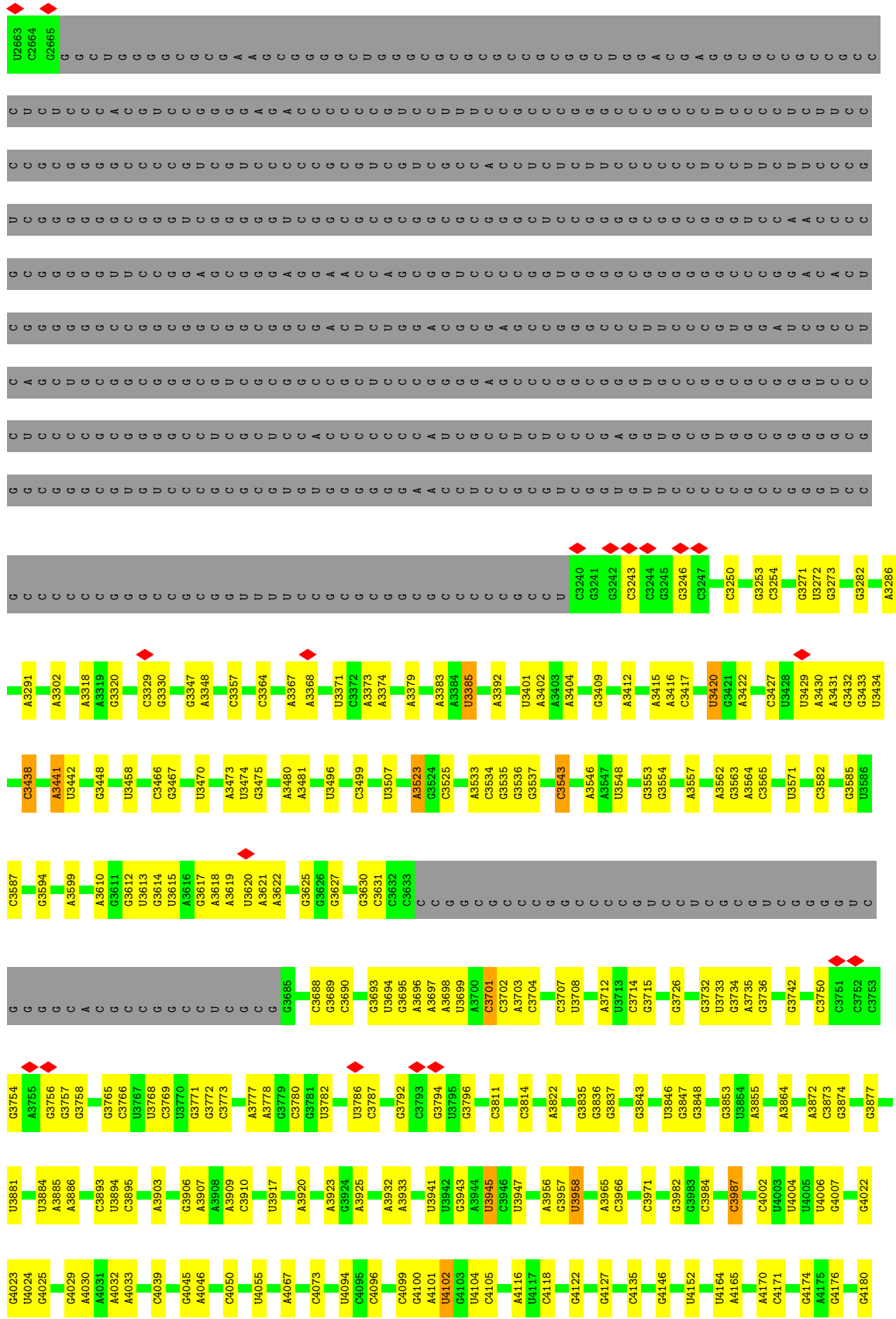
- Molecule 4: 60S ribosomal protein L10-like

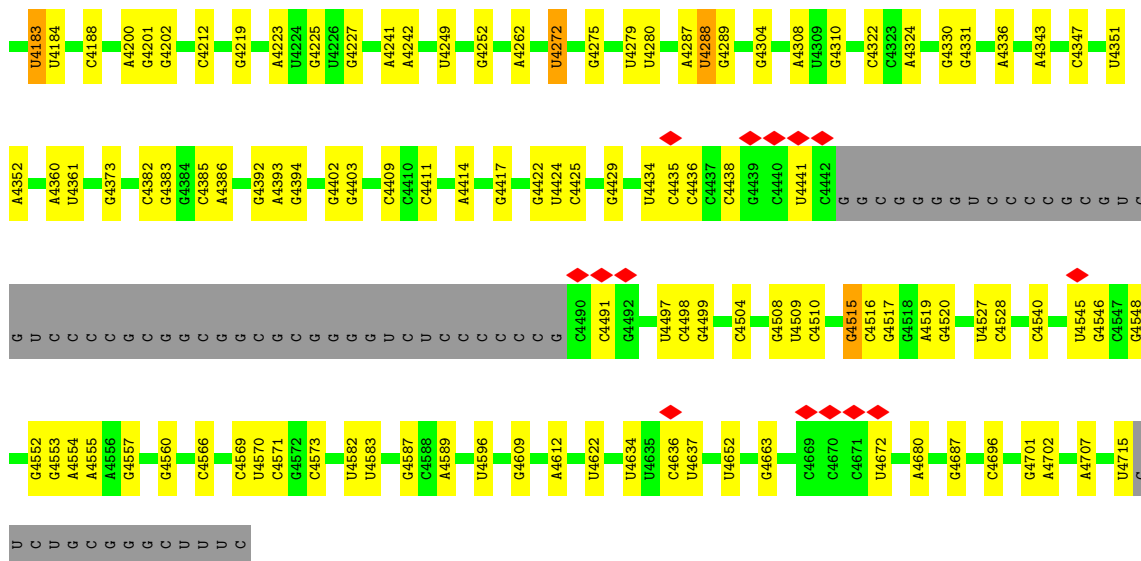


- Molecule 5: 60S ribosomal protein L11

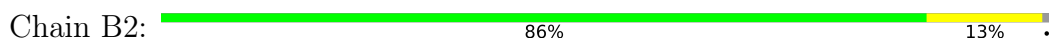




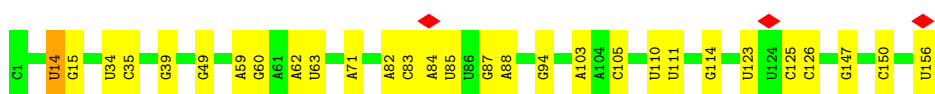
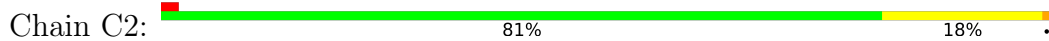




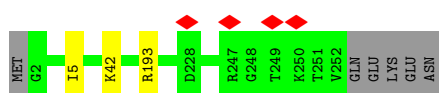
● Molecule 10: 5S rRNA



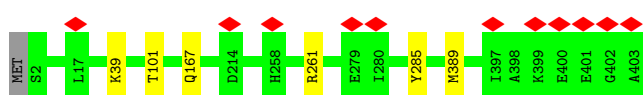
● Molecule 11: 5.8S rRNA



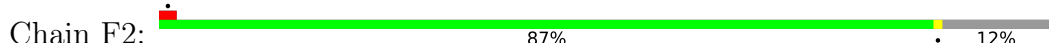
● Molecule 12: 60S ribosomal protein L8

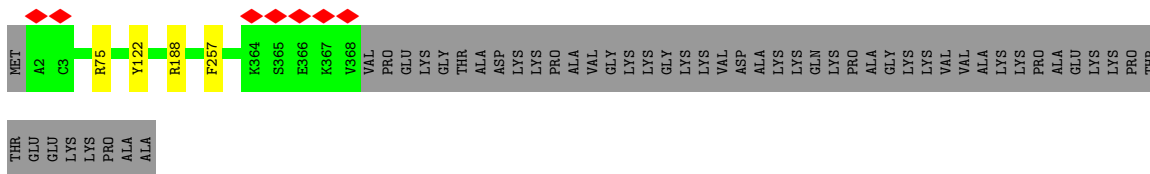


● Molecule 13: 60S ribosomal protein L3

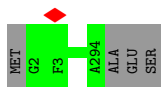


● Molecule 14: 60S ribosomal protein L4

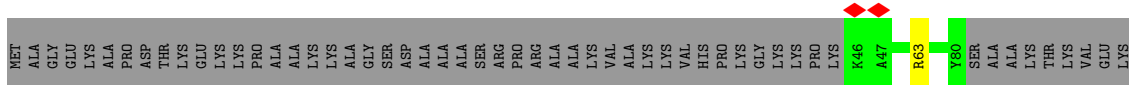
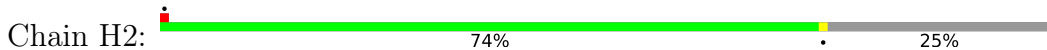




- Molecule 15: 60S ribosomal protein L5



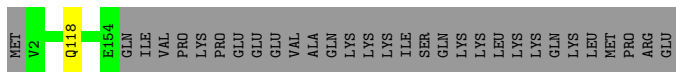
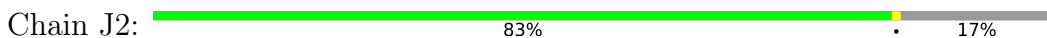
- Molecule 16: 60S ribosomal protein L6



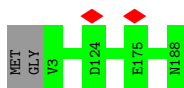
- Molecule 17: 60S ribosomal protein L13a



- Molecule 18: 60S ribosomal protein L17

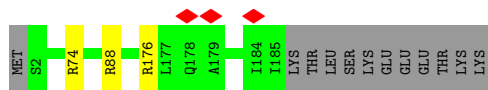


- Molecule 19: 60S ribosomal protein L18



- Molecule 20: 60S ribosomal protein L19





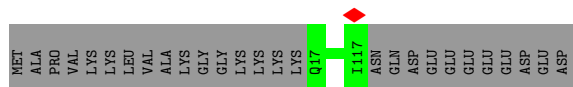
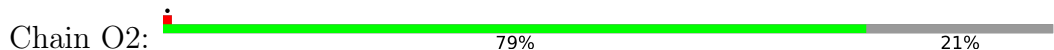
• Molecule 21: 60S ribosomal protein L18a



• Molecule 22: 60S ribosomal protein L21



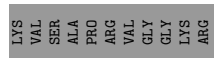
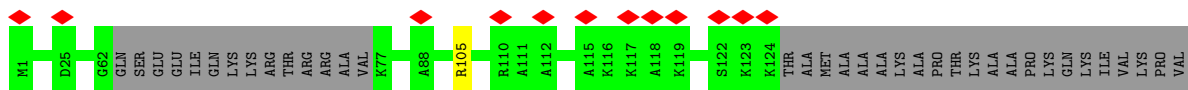
• Molecule 23: 60S ribosomal protein L22



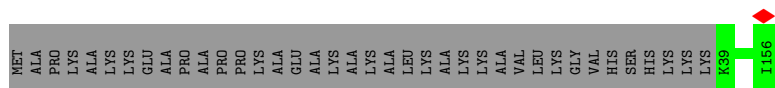
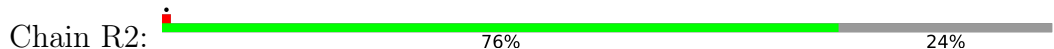
• Molecule 24: 60S ribosomal protein L23



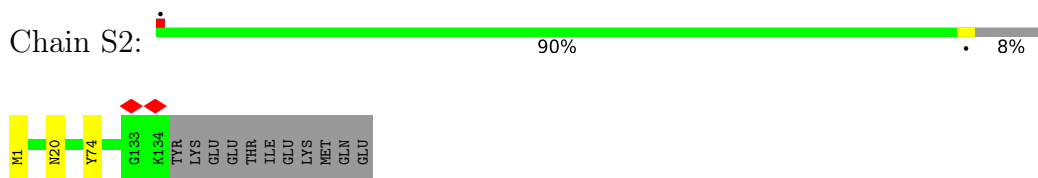
• Molecule 25: 60S ribosomal protein L24



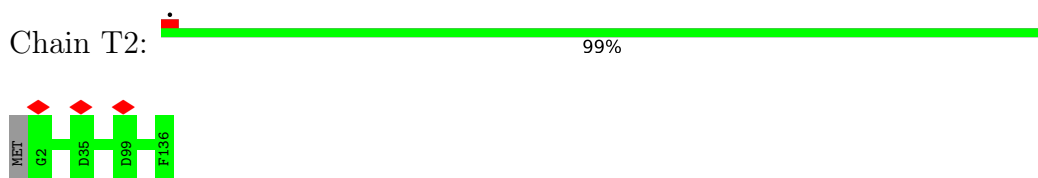
• Molecule 26: 60S ribosomal protein L23a



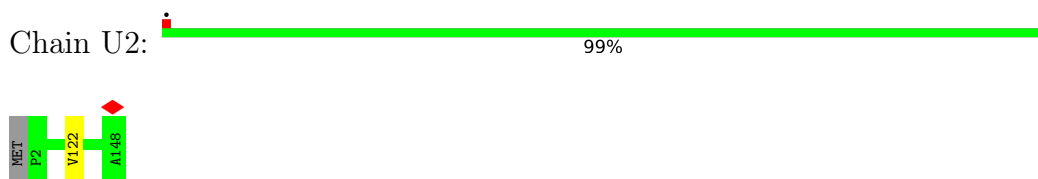
• Molecule 27: 60S ribosomal protein L26



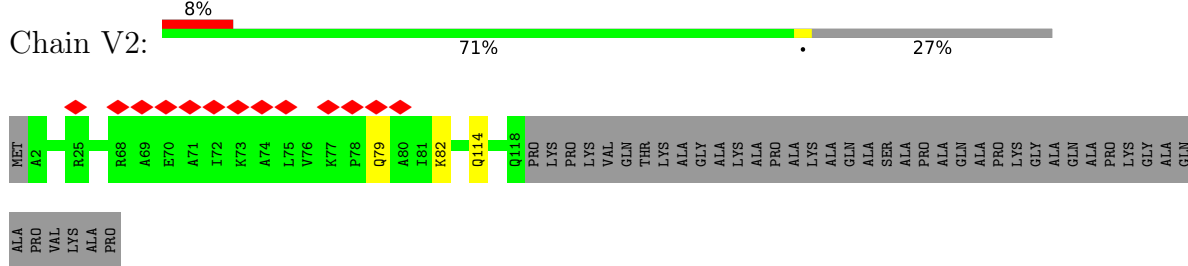
• Molecule 28: 60S ribosomal protein L27



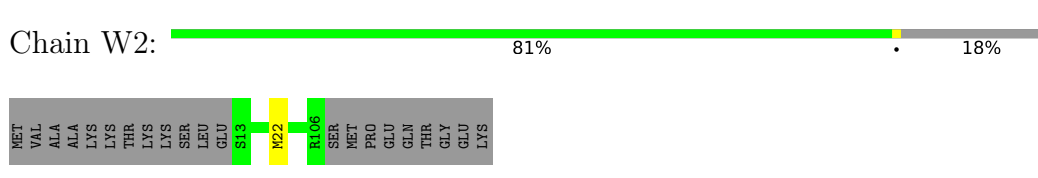
• Molecule 29: 60S ribosomal protein L27a



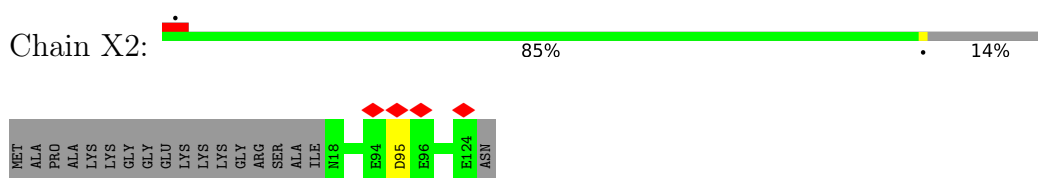
• Molecule 30: 60S ribosomal protein L29



• Molecule 31: 60S ribosomal protein L30

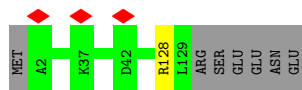


• Molecule 32: 60S ribosomal protein L31

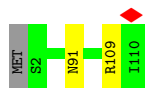


• Molecule 33: 60S ribosomal protein L32

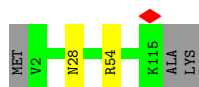




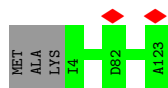
- Molecule 34: 60S ribosomal protein L35a



- Molecule 35: 60S ribosomal protein L34



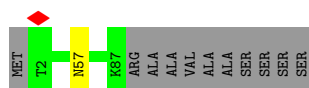
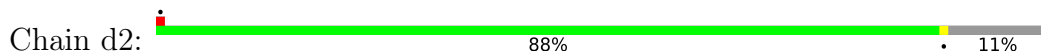
- Molecule 36: 60S ribosomal protein L35



- Molecule 37: 60S ribosomal protein L36



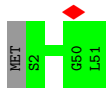
- Molecule 38: 60S ribosomal protein L37



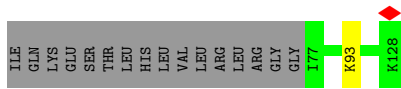
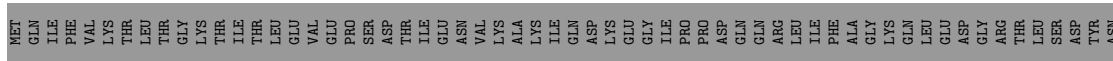
- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39



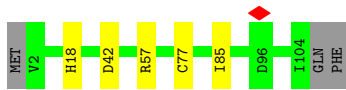
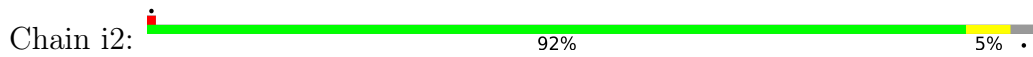
- Molecule 41: Ubiquitin-60S ribosomal protein L40



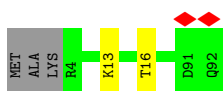
- Molecule 42: 60S ribosomal protein L41



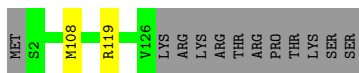
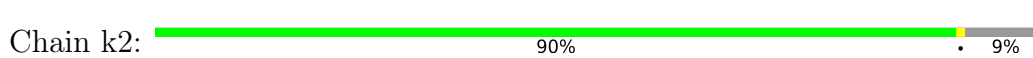
- Molecule 43: 60S ribosomal protein L36a



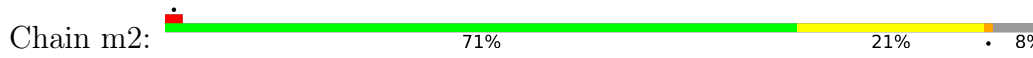
- Molecule 44: 60S ribosomal protein L37a

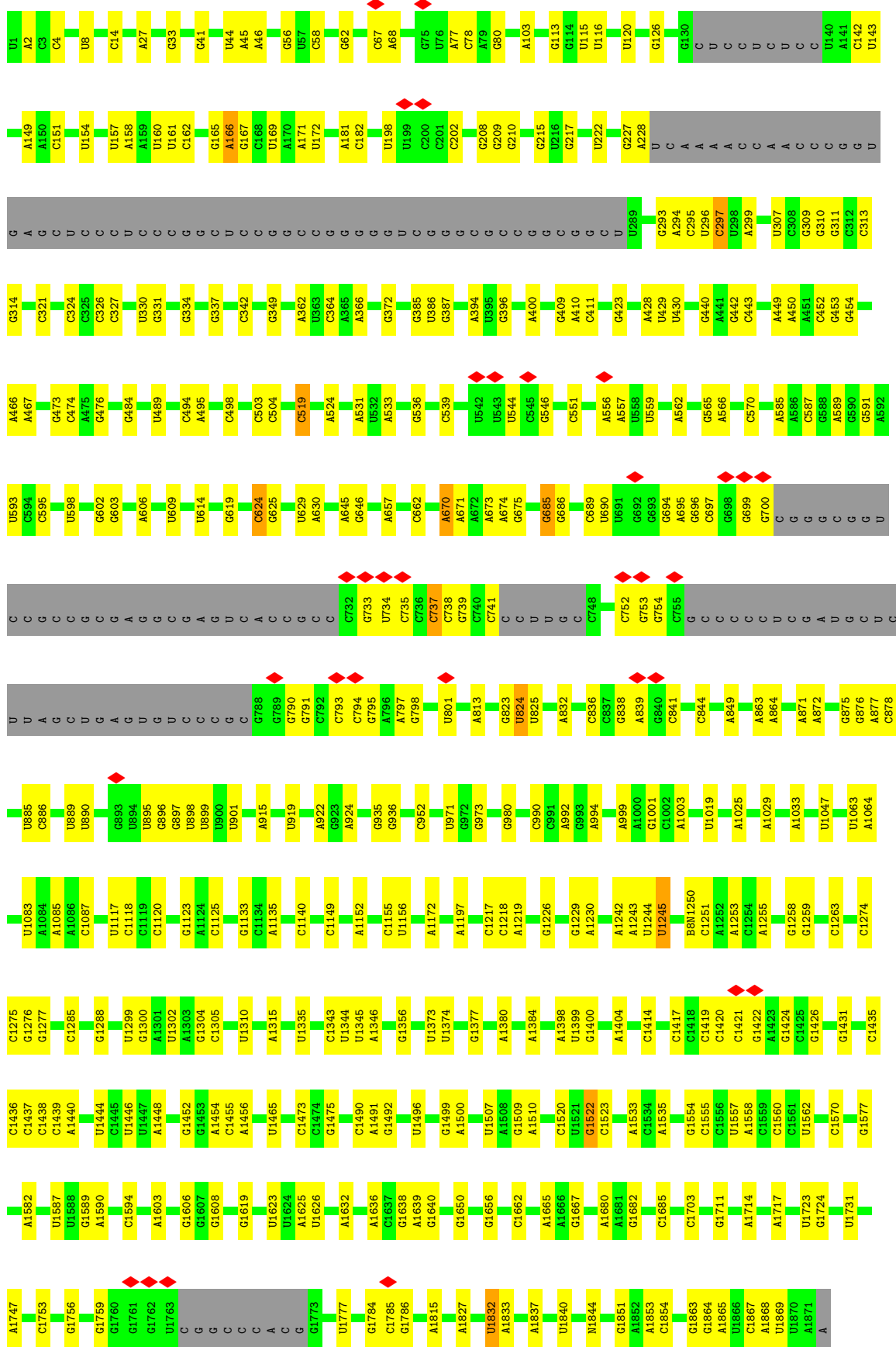


- Molecule 45: 60S ribosomal protein L28

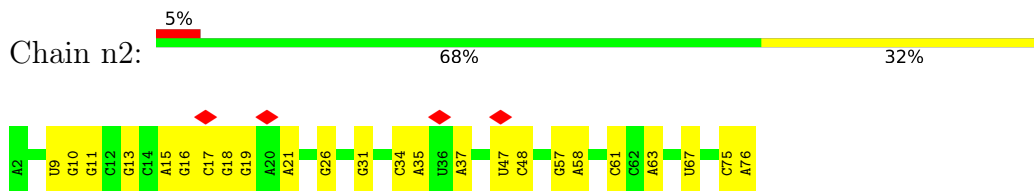


- Molecule 46: 18S rRNA

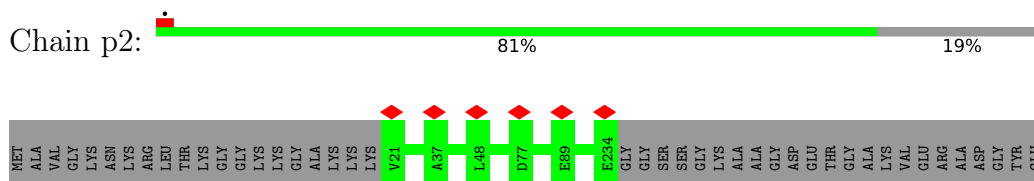




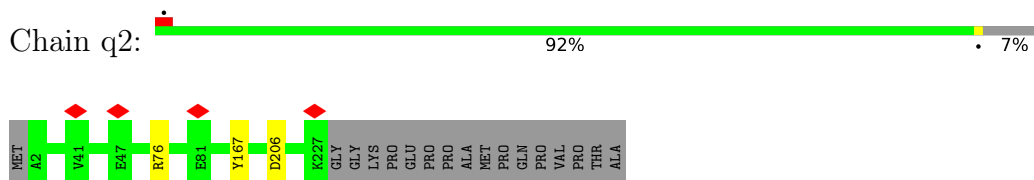
• Molecule 47: tRNA



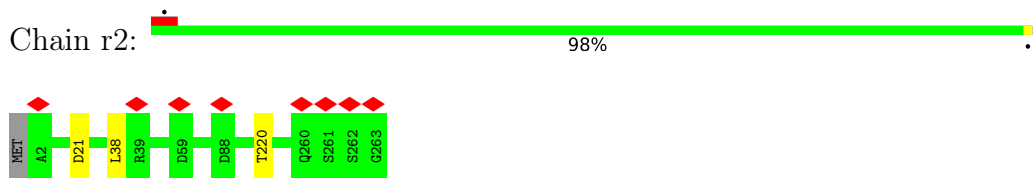
• Molecule 48: 40S ribosomal protein S3a



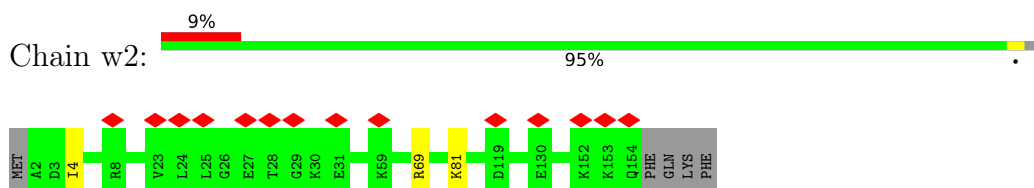
• Molecule 49: 40S ribosomal protein S3



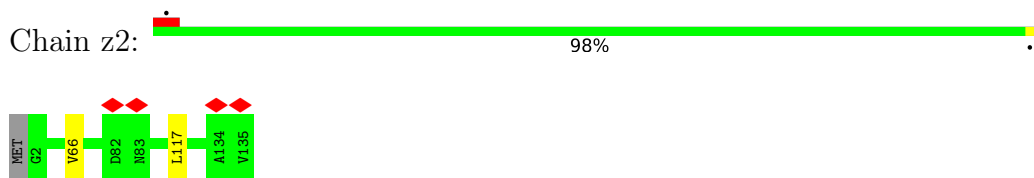
• Molecule 50: 40S ribosomal protein S4, X isoform



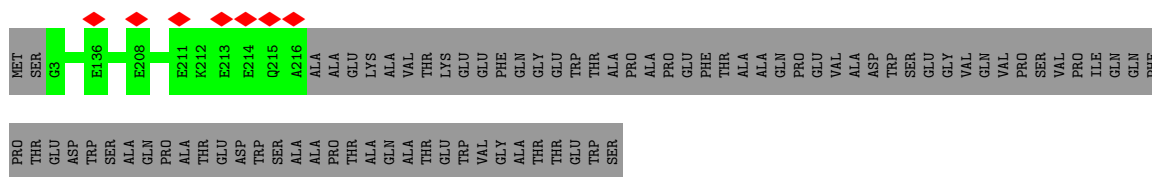
• Molecule 51: 40S ribosomal protein S11



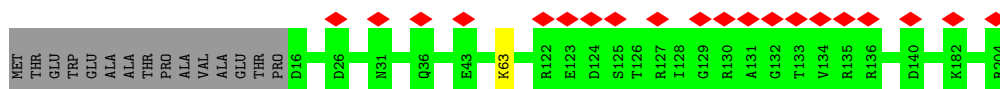
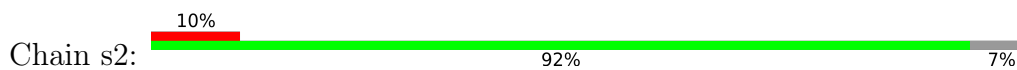
• Molecule 52: 40S ribosomal protein S17



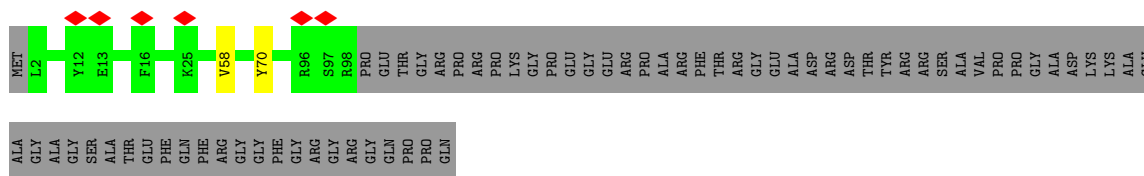
• Molecule 53: 40S ribosomal protein SA



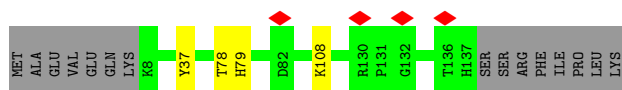
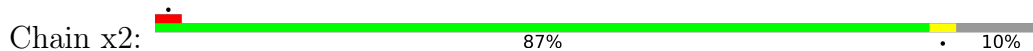
- Molecule 54: 40S ribosomal protein S5



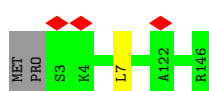
- Molecule 55: 40S ribosomal protein S10



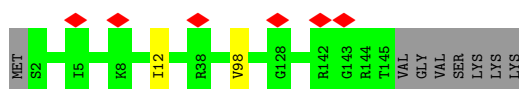
- Molecule 56: 40S ribosomal protein S15



- Molecule 57: 40S ribosomal protein S16



- Molecule 58: 40S ribosomal protein S18




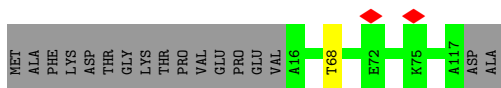
- Molecule 59: 40S ribosomal protein S19

Chain B3:  95%



- Molecule 60: 40S ribosomal protein S20

Chain C3:  85% 14%



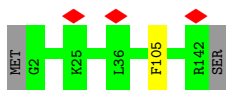
- Molecule 61: 40S ribosomal protein S21

Chain D3:  100%


There are no outlier residues recorded for this chain.

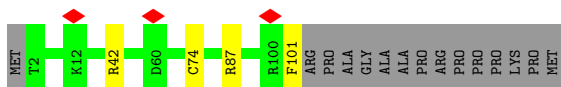
- Molecule 62: 40S ribosomal protein S23

Chain E3:  98%



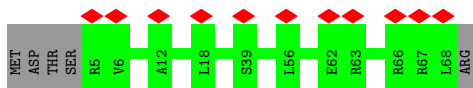
- Molecule 63: 40S ribosomal protein S26

Chain F3:  83% 13%



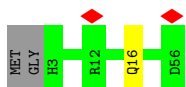
- Molecule 64: 40S ribosomal protein S28

Chain G3:  16% 93% 7%

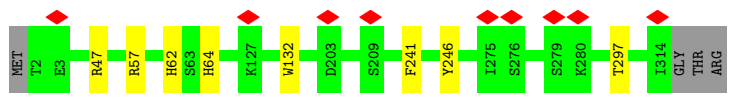


- Molecule 65: 40S ribosomal protein S29

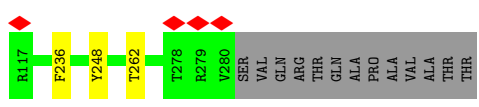
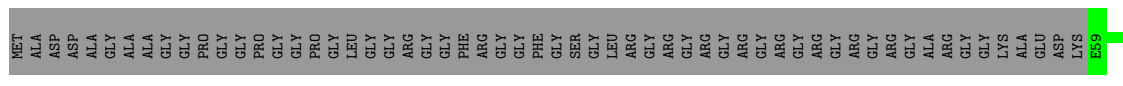
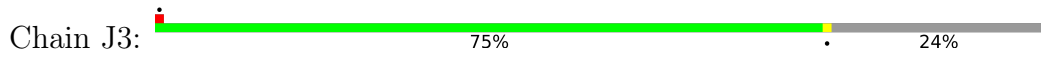
Chain H3:  95%



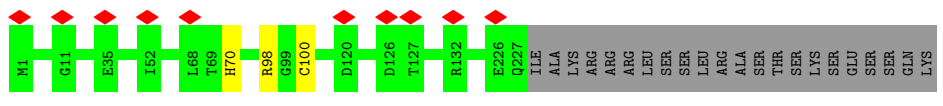
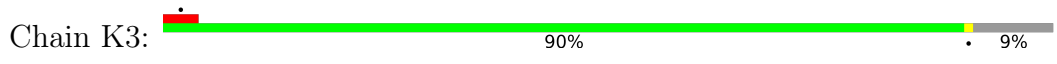
- Molecule 66: Receptor of activated protein C kinase 1



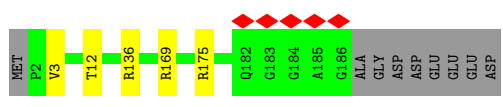
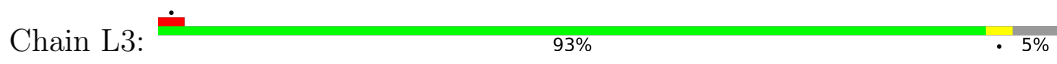
• Molecule 67: 40S ribosomal protein S2



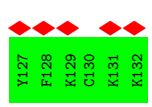
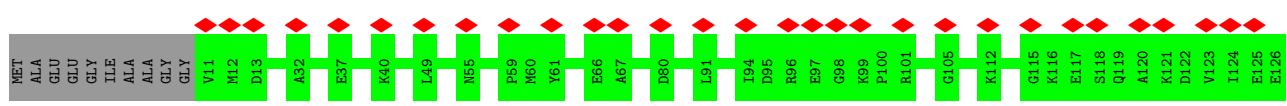
• Molecule 68: 40S ribosomal protein S6



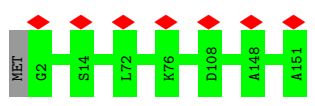
• Molecule 69: 40S ribosomal protein S9



• Molecule 70: 40S ribosomal protein S12

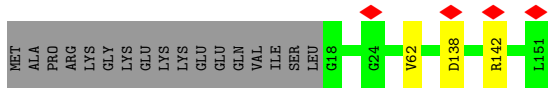


• Molecule 71: 40S ribosomal protein S13



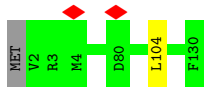
- Molecule 72: 40S ribosomal protein S14

Chain O3: 87% 11%



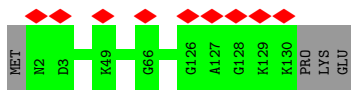
- Molecule 73: 40S ribosomal protein S15a

Chain P3: 98%



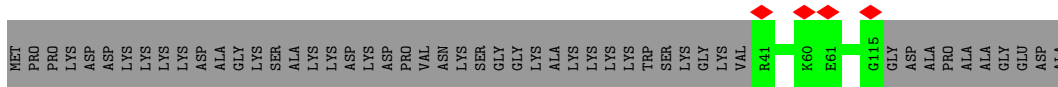
- Molecule 74: 40S ribosomal protein S24

Chain Q3: 7% 97%



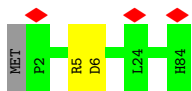
- Molecule 75: 40S ribosomal protein S25

Chain R3: 60% 40%



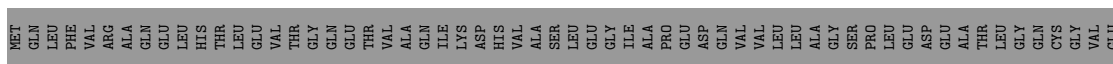
- Molecule 76: 40S ribosomal protein S27-like

Chain S3: 96%

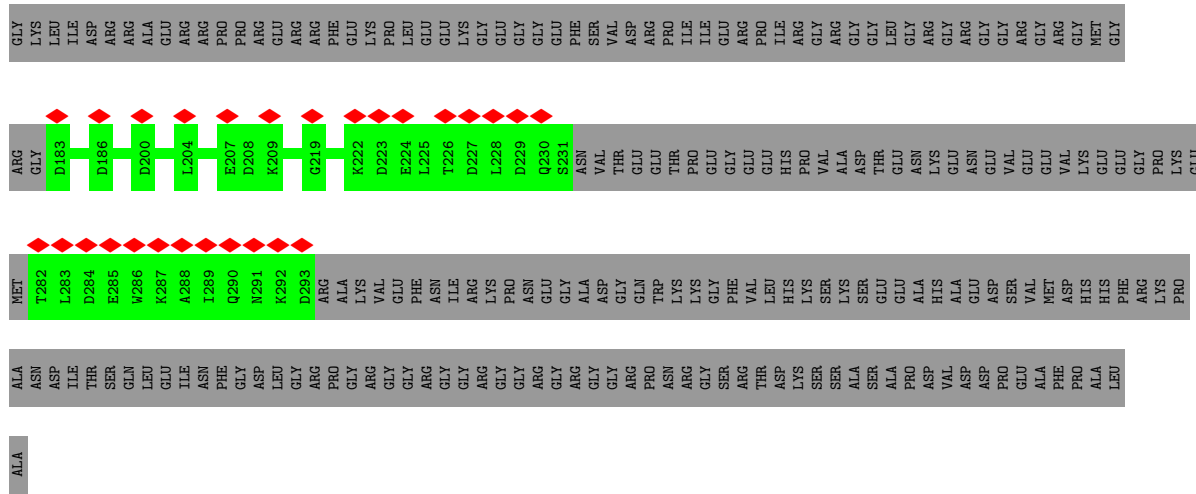


- Molecule 77: 40S ribosomal protein S30

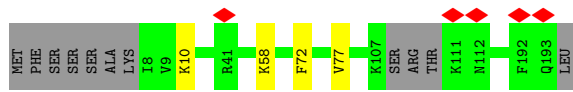
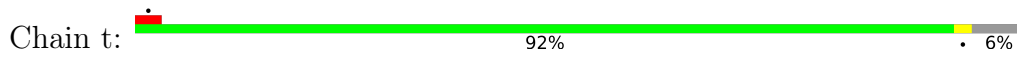
Chain T3: 41% 59%



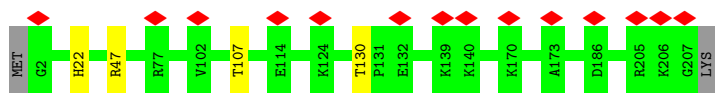
- Molecule 78: Ubiquitin-40S ribosomal protein S27a



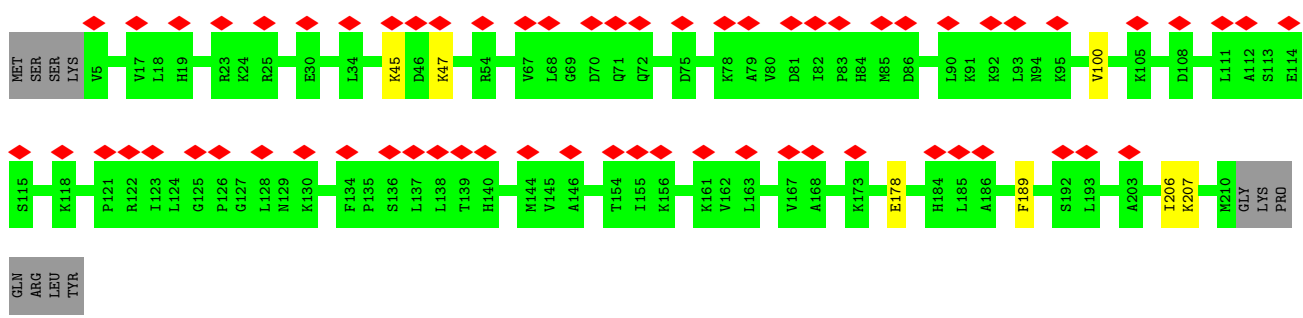
• Molecule 83: 40S ribosomal protein S7



• Molecule 84: 40S ribosomal protein S8



• Molecule 85: 60S ribosomal protein L10a



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23297	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 ($e^-/\text{\AA}^2$)	1.0	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	30.264	Depositor
Minimum map value	-17.005	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	1.034	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	814.07996, 814.07996, 814.07996	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, GDP, 6MZ, E6G, OMC, B8W, I4U, ZN, B8T, PSU, B9H, 4AC, MHG, P7G, A2M, 5MC, 1MA, OMG, B8Q, E7G, UR3, OMU, B8N, G7M, MG, DDE, MLZ, B9B

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A1	0.26	0/1888	0.51	0/2516
2	B1	0.24	0/1898	0.50	0/2553
3	C1	0.25	0/1537	0.51	0/2065
4	D1	0.25	0/1728	0.51	0/2306
5	E1	0.25	0/1420	0.53	0/1899
6	F1	0.25	0/1707	0.54	0/2286
7	G1	0.26	0/1165	0.51	0/1558
8	H1	0.25	0/1746	0.54	0/2338
9	A2	0.24	0/86883	0.79	28/135484 (0.0%)
10	B2	0.23	0/2858	0.79	0/4455
11	C2	0.23	0/3679	0.79	0/5732
12	D2	0.26	0/1959	0.55	0/2627
13	E2	0.25	0/3305	0.50	0/4422
14	F2	0.25	0/2971	0.52	0/3987
15	G2	0.25	0/2431	0.49	0/3256
16	H2	0.25	0/1822	0.51	0/2443
17	I2	0.26	0/1670	0.50	0/2232
18	J2	0.25	0/1268	0.51	0/1700
19	K2	0.25	0/1535	0.57	0/2048
20	L2	0.23	0/1558	0.52	0/2059
21	M2	0.26	0/1490	0.53	0/2000
22	N2	0.25	0/1326	0.50	0/1769
23	O2	0.25	0/839	0.49	0/1126
24	P2	0.26	0/983	0.49	0/1319
25	Q2	0.26	0/909	0.51	0/1203
26	R2	0.25	0/984	0.51	0/1323
27	S2	0.24	0/1132	0.52	0/1504
28	T2	0.26	0/1130	0.49	0/1507
29	U2	0.25	0/1193	0.51	0/1593
30	V2	0.24	0/963	0.47	0/1275
31	W2	0.25	0/742	0.46	0/996

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	X2	0.24	0/903	0.53	0/1216
33	Y2	0.24	0/1071	0.51	0/1429
34	Z2	0.26	0/895	0.55	0/1198
35	a2	0.24	0/916	0.55	0/1221
36	b2	0.24	0/1009	0.51	0/1332
37	c2	0.24	0/838	0.53	0/1111
38	d2	0.25	0/720	0.57	0/952
39	e2	0.24	0/574	0.47	0/760
40	f2	0.24	0/454	0.54	0/599
41	g2	0.23	0/425	0.52	0/561
42	h2	0.23	0/231	0.67	0/294
43	i2	0.25	0/855	0.53	0/1128
44	j2	0.25	0/704	0.49	0/935
45	k2	0.24	0/1016	0.54	0/1363
46	m2	0.22	0/40772	0.79	12/63546 (0.0%)
47	n2	0.22	0/1795	0.80	0/2798
48	p2	0.24	0/1765	0.47	0/2362
49	q2	0.25	0/1784	0.50	0/2402
50	r2	0.25	0/2118	0.50	0/2849
51	w2	0.25	0/1268	0.53	0/1696
52	z2	0.23	0/1094	0.49	0/1469
53	o2	0.24	0/1731	0.48	0/2352
54	s2	0.23	0/1517	0.48	0/2038
55	v2	0.24	0/843	0.44	0/1137
56	x2	0.25	0/1094	0.51	0/1460
57	y2	0.25	0/1161	0.52	0/1553
58	A3	0.23	0/1208	0.55	0/1618
59	B3	0.24	0/1122	0.48	0/1503
60	C3	0.23	0/817	0.53	0/1097
61	D3	0.26	0/645	0.50	0/863
62	E3	0.25	0/1116	0.51	0/1490
63	F3	0.25	0/828	0.55	0/1109
64	G3	0.24	0/508	0.59	0/680
65	H3	0.25	0/466	0.51	0/618
66	I3	0.24	0/2493	0.50	0/3394
67	J3	0.25	0/1762	0.47	0/2382
68	K3	0.24	0/1863	0.53	0/2481
69	L3	0.24	0/1550	0.53	0/2069
70	M3	0.23	0/952	0.42	0/1278
71	N3	0.23	0/1232	0.47	0/1656
72	O3	0.25	0/1015	0.53	0/1361
73	P3	0.25	0/1051	0.52	0/1406
74	Q3	0.24	0/1066	0.50	0/1415

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	R3	0.24	0/604	0.50	0/810
76	S3	0.24	0/665	0.49	0/890
77	T3	0.25	0/443	0.54	0/582
78	U3	0.25	0/515	0.50	0/682
79	m	0.25	0/6756	0.47	0/9122
80	j	0.24	0/1530	0.46	0/2064
81	k	0.23	0/1173	0.49	0/1581
82	A	0.23	0/493	0.51	0/655
83	t	0.25	0/1499	0.47	0/2007
84	u	0.24	0/1715	0.52	0/2287
85	L1	0.24	0/1686	0.49	0/2262
All	All	0.24	0/241045	0.69	40/352704 (0.0%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	m2	624	C	N3-C2-O2	-8.27	116.11	121.90
46	m2	1149	C	N3-C2-O2	-8.18	116.18	121.90
9	A2	260	C	N3-C2-O2	-7.97	116.32	121.90
9	A2	822	C	N3-C2-O2	-7.77	116.46	121.90
9	A2	1893	C	C2-N1-C1'	7.24	126.77	118.80
46	m2	737	C	N3-C2-O2	-7.21	116.85	121.90
9	A2	112	C	C2-N1-C1'	7.00	126.50	118.80
46	m2	297	C	N3-C2-O2	-6.93	117.05	121.90
9	A2	1893	C	N1-C2-O2	6.63	122.88	118.90
46	m2	737	C	N1-C2-O2	6.47	122.78	118.90
9	A2	112	C	N1-C2-O2	6.24	122.64	118.90
46	m2	603	G	C5-C6-O6	6.22	132.33	128.60
9	A2	180	C	N1-C2-O2	6.21	122.62	118.90
46	m2	1263	C	N1-C2-O2	5.99	122.50	118.90
9	A2	3811	C	N3-C2-O2	-5.98	117.72	121.90
46	m2	1522	G	C4-N9-C1'	5.95	134.23	126.50
9	A2	4122	G	N1-C6-O6	-5.90	116.36	119.90
46	m2	1263	C	C2-N1-C1'	5.88	125.27	118.80
9	A2	260	C	N1-C2-O2	5.88	122.43	118.90
46	m2	1149	C	N1-C2-O2	5.80	122.38	118.90
9	A2	155	C	N3-C2-O2	-5.80	117.84	121.90
9	A2	131	C	C2-N1-C1'	5.75	125.13	118.80
9	A2	2283	G	C4-N9-C1'	5.69	133.89	126.50
9	A2	932	C	N3-C2-O2	-5.55	118.01	121.90
9	A2	931	C	N1-C2-O2	5.51	122.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	3701	C	N3-C2-O2	-5.51	118.05	121.90
9	A2	1893	C	C6-N1-C1'	-5.46	114.24	120.80
46	m2	1125	C	N3-C2-O2	-5.39	118.12	121.90
46	m2	603	G	N1-C6-O6	-5.37	116.68	119.90
9	A2	326	C	N3-C2-O2	-5.33	118.17	121.90
9	A2	26	C	N1-C2-O2	5.27	122.06	118.90
9	A2	112	C	C6-N1-C1'	-5.24	114.51	120.80
9	A2	155	C	N1-C2-O2	5.20	122.02	118.90
9	A2	932	C	C6-N1-C2	-5.16	118.23	120.30
9	A2	256	G	N3-C2-N2	5.08	123.46	119.90
9	A2	180	C	N3-C2-O2	-5.07	118.36	121.90
9	A2	256	G	N1-C2-N2	-5.05	111.65	116.20
9	A2	3750	C	N1-C2-O2	5.05	121.93	118.90
9	A2	2507	G	C4-N9-C1'	5.03	133.04	126.50
9	A2	3811	C	N1-C2-O2	5.02	121.91	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	221/270 (82%)	214 (97%)	7 (3%)	0	100	100
2	B1	227/266 (85%)	220 (97%)	7 (3%)	0	100	100
3	C1	188/192 (98%)	185 (98%)	3 (2%)	0	100	100
4	D1	204/214 (95%)	201 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E1	172/178 (97%)	167 (97%)	5 (3%)	0	100	100
6	F1	205/211 (97%)	194 (95%)	11 (5%)	0	100	100
7	G1	137/217 (63%)	133 (97%)	4 (3%)	0	100	100
8	H1	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
12	D2	249/257 (97%)	234 (94%)	15 (6%)	0	100	100
13	E2	400/403 (99%)	397 (99%)	3 (1%)	0	100	100
14	F2	364/419 (87%)	359 (99%)	5 (1%)	0	100	100
15	G2	291/297 (98%)	284 (98%)	7 (2%)	0	100	100
16	H2	215/296 (73%)	208 (97%)	7 (3%)	0	100	100
17	I2	199/203 (98%)	195 (98%)	4 (2%)	0	100	100
18	J2	151/184 (82%)	146 (97%)	5 (3%)	0	100	100
19	K2	184/188 (98%)	181 (98%)	3 (2%)	0	100	100
20	L2	182/196 (93%)	181 (100%)	1 (0%)	0	100	100
21	M2	173/176 (98%)	166 (96%)	7 (4%)	0	100	100
22	N2	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
23	O2	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
24	P2	127/140 (91%)	125 (98%)	2 (2%)	0	100	100
25	Q2	106/157 (68%)	104 (98%)	2 (2%)	0	100	100
26	R2	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
27	S2	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
28	T2	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
29	U2	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
30	V2	115/160 (72%)	110 (96%)	5 (4%)	0	100	100
31	W2	92/115 (80%)	86 (94%)	6 (6%)	0	100	100
32	X2	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
33	Y2	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
34	Z2	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
35	a2	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
36	b2	118/123 (96%)	115 (98%)	3 (2%)	0	100	100
37	c2	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
38	d2	84/97 (87%)	82 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	e2	67/70 (96%)	67 (100%)	0	0	100	100
40	f2	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
41	g2	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
42	h2	22/25 (88%)	22 (100%)	0	0	100	100
43	i2	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
44	j2	87/92 (95%)	83 (95%)	4 (5%)	0	100	100
45	k2	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
48	p2	212/264 (80%)	210 (99%)	2 (1%)	0	100	100
49	q2	224/243 (92%)	217 (97%)	7 (3%)	0	100	100
50	r2	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
51	w2	151/158 (96%)	144 (95%)	7 (5%)	0	100	100
52	z2	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
53	o2	212/295 (72%)	211 (100%)	1 (0%)	0	100	100
54	s2	187/204 (92%)	182 (97%)	5 (3%)	0	100	100
55	v2	95/165 (58%)	93 (98%)	2 (2%)	0	100	100
56	x2	128/145 (88%)	124 (97%)	3 (2%)	1 (1%)	19	54
57	y2	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
58	A3	142/152 (93%)	138 (97%)	4 (3%)	0	100	100
59	B3	139/145 (96%)	139 (100%)	0	0	100	100
60	C3	100/119 (84%)	97 (97%)	3 (3%)	0	100	100
61	D3	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
62	E3	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
63	F3	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
64	G3	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
65	H3	52/56 (93%)	50 (96%)	2 (4%)	0	100	100
66	I3	311/317 (98%)	295 (95%)	16 (5%)	0	100	100
67	J3	220/293 (75%)	217 (99%)	3 (1%)	0	100	100
68	K3	225/249 (90%)	223 (99%)	2 (1%)	0	100	100
69	L3	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
70	M3	120/132 (91%)	114 (95%)	6 (5%)	0	100	100
71	N3	148/151 (98%)	144 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	O3	132/151 (87%)	126 (96%)	6 (4%)	0	100	100
73	P3	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
74	Q3	127/133 (96%)	122 (96%)	5 (4%)	0	100	100
75	R3	73/125 (58%)	73 (100%)	0	0	100	100
76	S3	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
77	T3	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
78	U3	60/156 (38%)	59 (98%)	1 (2%)	0	100	100
79	m	846/858 (99%)	823 (97%)	23 (3%)	0	100	100
80	j	194/317 (61%)	191 (98%)	3 (2%)	0	100	100
81	k	151/165 (92%)	144 (95%)	6 (4%)	1 (1%)	22	57
82	A	57/386 (15%)	57 (100%)	0	0	100	100
83	t	179/194 (92%)	174 (97%)	5 (3%)	0	100	100
84	u	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
85	L1	204/217 (94%)	187 (92%)	16 (8%)	1 (0%)	29	64
All	All	12686/14730 (86%)	12350 (97%)	333 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
81	k	147	HIS
56	x2	108	LYS
85	L1	207	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	194/234 (83%)	194 (100%)	0	100	100
2	B1	198/223 (89%)	197 (100%)	1 (0%)	88	94
3	C1	169/171 (99%)	168 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D1	177/180 (98%)	174 (98%)	3 (2%)	60	83
5	E1	147/149 (99%)	142 (97%)	5 (3%)	37	69
6	F1	174/178 (98%)	169 (97%)	5 (3%)	42	72
7	G1	118/157 (75%)	118 (100%)	0	100	100
8	H1	171/172 (99%)	168 (98%)	3 (2%)	59	82
12	D2	193/199 (97%)	190 (98%)	3 (2%)	62	84
13	E2	347/348 (100%)	341 (98%)	6 (2%)	60	83
14	F2	307/347 (88%)	303 (99%)	4 (1%)	69	87
15	G2	245/249 (98%)	245 (100%)	0	100	100
16	H2	198/256 (77%)	196 (99%)	2 (1%)	76	90
17	I2	172/173 (99%)	169 (98%)	3 (2%)	60	83
18	J2	134/164 (82%)	133 (99%)	1 (1%)	84	93
19	K2	164/165 (99%)	164 (100%)	0	100	100
20	L2	163/175 (93%)	160 (98%)	3 (2%)	59	82
21	M2	155/156 (99%)	154 (99%)	1 (1%)	86	94
22	N2	138/139 (99%)	136 (99%)	2 (1%)	67	86
23	O2	91/114 (80%)	91 (100%)	0	100	100
24	P2	100/107 (94%)	99 (99%)	1 (1%)	76	90
25	Q2	90/126 (71%)	89 (99%)	1 (1%)	73	89
26	R2	106/133 (80%)	106 (100%)	0	100	100
27	S2	124/135 (92%)	121 (98%)	3 (2%)	49	76
28	T2	117/118 (99%)	117 (100%)	0	100	100
29	U2	120/121 (99%)	119 (99%)	1 (1%)	81	92
30	V2	98/124 (79%)	95 (97%)	3 (3%)	40	70
31	W2	79/97 (81%)	78 (99%)	1 (1%)	69	87
32	X2	98/110 (89%)	97 (99%)	1 (1%)	76	90
33	Y2	114/121 (94%)	113 (99%)	1 (1%)	78	91
34	Z2	88/89 (99%)	86 (98%)	2 (2%)	50	77
35	a2	98/100 (98%)	96 (98%)	2 (2%)	55	80
36	b2	108/110 (98%)	108 (100%)	0	100	100
37	c2	86/90 (96%)	85 (99%)	1 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	d2	73/80 (91%)	72 (99%)	1 (1%)	67	86
39	e2	64/65 (98%)	64 (100%)	0	100	100
40	f2	47/48 (98%)	47 (100%)	0	100	100
41	g2	47/115 (41%)	46 (98%)	1 (2%)	53	79
42	h2	23/24 (96%)	23 (100%)	0	100	100
43	i2	91/94 (97%)	86 (94%)	5 (6%)	21	53
44	j2	73/75 (97%)	71 (97%)	2 (3%)	44	74
45	k2	109/121 (90%)	107 (98%)	2 (2%)	59	82
48	p2	195/229 (85%)	195 (100%)	0	100	100
49	q2	189/202 (94%)	186 (98%)	3 (2%)	62	84
50	r2	224/225 (100%)	221 (99%)	3 (1%)	69	87
51	w2	137/142 (96%)	134 (98%)	3 (2%)	52	78
52	z2	120/121 (99%)	118 (98%)	2 (2%)	60	83
53	o2	179/242 (74%)	179 (100%)	0	100	100
54	s2	159/170 (94%)	158 (99%)	1 (1%)	86	94
55	v2	88/136 (65%)	86 (98%)	2 (2%)	50	77
56	x2	116/130 (89%)	113 (97%)	3 (3%)	46	74
57	y2	119/121 (98%)	118 (99%)	1 (1%)	81	92
58	A3	125/132 (95%)	123 (98%)	2 (2%)	62	84
59	B3	112/115 (97%)	109 (97%)	3 (3%)	44	74
60	C3	93/107 (87%)	92 (99%)	1 (1%)	73	89
61	D3	67/67 (100%)	67 (100%)	0	100	100
62	E3	113/115 (98%)	112 (99%)	1 (1%)	78	91
63	F3	88/98 (90%)	84 (96%)	4 (4%)	27	60
64	G3	57/62 (92%)	57 (100%)	0	100	100
65	H3	48/49 (98%)	47 (98%)	1 (2%)	53	79
66	I3	272/275 (99%)	264 (97%)	8 (3%)	42	72
67	J3	188/224 (84%)	185 (98%)	3 (2%)	62	84
68	K3	198/218 (91%)	195 (98%)	3 (2%)	65	85
69	L3	161/168 (96%)	156 (97%)	5 (3%)	40	70
70	M3	102/108 (94%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	N3	130/131 (99%)	130 (100%)	0	100	100
72	O3	104/119 (87%)	101 (97%)	3 (3%)	42	72
73	P3	112/113 (99%)	111 (99%)	1 (1%)	78	91
74	Q3	111/115 (96%)	111 (100%)	0	100	100
75	R3	66/103 (64%)	66 (100%)	0	100	100
76	S3	75/76 (99%)	73 (97%)	2 (3%)	44	74
77	T3	45/106 (42%)	44 (98%)	1 (2%)	52	78
78	U3	55/140 (39%)	51 (93%)	4 (7%)	14	43
79	m	725/729 (100%)	711 (98%)	14 (2%)	57	81
80	j	164/255 (64%)	160 (98%)	4 (2%)	49	76
81	k	126/137 (92%)	121 (96%)	5 (4%)	31	65
82	A	52/304 (17%)	52 (100%)	0	100	100
83	t	164/174 (94%)	160 (98%)	4 (2%)	49	76
84	u	178/180 (99%)	174 (98%)	4 (2%)	52	78
85	L1	187/197 (95%)	181 (97%)	6 (3%)	39	69
All	All	11052/12487 (88%)	10884 (98%)	168 (2%)	66	85

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B1	175	ARG
3	C1	173	ARG
4	D1	10	ARG
4	D1	21	ARG
4	D1	24	ARG
5	E1	22	LEU
5	E1	33	LEU
5	E1	90	ARG
5	E1	115	LEU
5	E1	146	ARG
6	F1	59	VAL
6	F1	63	THR
6	F1	67	HIS
6	F1	136	LYS
6	F1	162	LYS
8	H1	140	LYS
8	H1	193	ARG

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Mol	Chain	Res	Type
8	H1	204	ARG
12	D2	5	ILE
12	D2	42	LYS
12	D2	193	ARG
13	E2	39	LYS
13	E2	101	THR
13	E2	167	GLN
13	E2	261	ARG
13	E2	285	TYR
13	E2	389	MET
14	F2	75	ARG
14	F2	122	TYR
14	F2	188	ARG
14	F2	257	PHE
16	H2	63	ARG
16	H2	201	VAL
17	I2	117	ARG
17	I2	149	TYR
17	I2	190	CYS
18	J2	118	GLN
20	L2	74	ARG
20	L2	88	ARG
20	L2	176	ARG
21	M2	32	ILE
22	N2	76	VAL
22	N2	81	LYS
24	P2	72	LEU
25	Q2	105	ARG
27	S2	1	MET
27	S2	20	ASN
27	S2	74	TYR
29	U2	122	VAL
30	V2	79	GLN
30	V2	82	LYS
30	V2	114	GLN
31	W2	22	MET
32	X2	95	ASP
33	Y2	128	ARG
34	Z2	91	ASN
34	Z2	109	ARG
35	a2	28	ASN
35	a2	54	ARG

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Mol	Chain	Res	Type
37	c2	29	ARG
38	d2	57	ASN
41	g2	93	LYS
43	i2	18	HIS
43	i2	42	ASP
43	i2	57	ARG
43	i2	77	CYS
43	i2	85	ILE
44	j2	13	LYS
44	j2	16	THR
45	k2	108	MET
45	k2	119	ARG
49	q2	76	ARG
49	q2	167	TYR
49	q2	206	ASP
50	r2	21	ASP
50	r2	38	LEU
50	r2	220	THR
51	w2	4	ILE
51	w2	69	ARG
51	w2	81	LYS
52	z2	66	VAL
52	z2	117	LEU
54	s2	63	LYS
55	v2	58	VAL
55	v2	70	TYR
56	x2	37	TYR
56	x2	78	THR
56	x2	79	HIS
57	y2	7	LEU
58	A3	12	ILE
58	A3	98	VAL
59	B3	33	TRP
59	B3	64	LEU
59	B3	129	ARG
60	C3	68	THR
62	E3	105	PHE
63	F3	42	ARG
63	F3	74	CYS
63	F3	87	ARG
63	F3	101	PHE
65	H3	16	GLN

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Mol	Chain	Res	Type
66	I3	47	ARG
66	I3	57	ARG
66	I3	62	HIS
66	I3	64	HIS
66	I3	132	TRP
66	I3	241	PHE
66	I3	246	TYR
66	I3	297	THR
67	J3	236	PHE
67	J3	248	TYR
67	J3	262	THR
68	K3	70	HIS
68	K3	98	ARG
68	K3	100	CYS
69	L3	3	VAL
69	L3	12	THR
69	L3	136	ARG
69	L3	169	ARG
69	L3	175	ARG
72	O3	62	VAL
72	O3	138	ASP
72	O3	142	ARG
73	P3	104	LEU
76	S3	5	ARG
76	S3	6	ASP
77	T3	46	VAL
78	U3	116	ARG
78	U3	117	LEU
78	U3	118	ARG
78	U3	138	ARG
79	m	3	PHE
79	m	29	HIS
79	m	49	ARG
79	m	70	LYS
79	m	76	LEU
79	m	77	PHE
79	m	225	LYS
79	m	263	ARG
79	m	372	TYR
79	m	455	ARG
79	m	530	ASP
79	m	744	TYR

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Mol	Chain	Res	Type
79	m	745	LEU
79	m	817	GLN
80	j	30	VAL
80	j	70	GLU
80	j	100	ASP
80	j	160	LEU
81	k	16	ARG
81	k	70	GLN
81	k	143	VAL
81	k	147	HIS
81	k	156	ASN
83	t	10	LYS
83	t	58	LYS
83	t	72	PHE
83	t	77	VAL
84	u	22	HIS
84	u	47	ARG
84	u	107	THR
84	u	130	THR
85	L1	45	LYS
85	L1	47	LYS
85	L1	100	VAL
85	L1	178	GLU
85	L1	189	PHE
85	L1	206	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
33	Y2	43	ASN
54	s2	179	ASN
61	D3	35	ASN
67	J3	267	GLN
69	L3	111	GLN
73	P3	91	ASN
74	Q3	94	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B2	119/121 (98%)	16 (13%)	0
11	C2	155/156 (99%)	28 (18%)	2 (1%)
46	m2	1715/1871 (91%)	385 (22%)	0
47	n2	74/75 (98%)	24 (32%)	0
9	A2	3676/4731 (77%)	784 (21%)	13 (0%)
All	All	5739/6954 (82%)	1237 (21%)	15 (0%)

All (1237) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A2	2	G
9	A2	25	A
9	A2	39	A
9	A2	42	A
9	A2	48	G
9	A2	59	A
9	A2	64	A
9	A2	65	A
9	A2	66	A
9	A2	73	A
9	A2	76	A
9	A2	91	G
9	A2	95	G
9	A2	104	G
9	A2	106	A
9	A2	109	G
9	A2	116	G
9	A2	119	G
9	A2	120	A
9	A2	133	C
9	A2	134	G
9	A2	136	C
9	A2	137	G
9	A2	138	C
9	A2	143	U
9	A2	144	G
9	A2	158	A
9	A2	159	C
9	A2	164	G
9	A2	171	U
9	A2	172	C
9	A2	178	C
9	A2	179	G

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Mol	Chain	Res	Type
9	A2	183	C
9	A2	184	U
9	A2	185	C
9	A2	187	U
9	A2	188	G
9	A2	189	G
9	A2	197	A
9	A2	200	U
9	A2	201	C
9	A2	209	U
9	A2	216	C
9	A2	217	C
9	A2	218	A
9	A2	233	U
9	A2	234	G
9	A2	238	C
9	A2	254	G
9	A2	258	G
9	A2	259	C
9	A2	265	U
9	A2	266	C
9	A2	267	G
9	A2	269	G
9	A2	274	C
9	A2	278	G
9	A2	280	G
9	A2	297	U
9	A2	315	G
9	A2	316	U
9	A2	328	A
9	A2	330	G
9	A2	340	C
9	A2	341	G
9	A2	345	C
9	A2	373	OMG
9	A2	387	G
9	A2	396	A
9	A2	398	A2M
9	A2	399	G
9	A2	407	A
9	A2	409	G
9	A2	410	A

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Mol	Chain	Res	Type
9	A2	412	G
9	A2	413	G
9	A2	418	A
9	A2	433	A
9	A2	439	G
9	A2	440	U
9	A2	450	G
9	A2	452	A
9	A2	453	G
9	A2	454	U
9	A2	456	C
9	A2	457	G
9	A2	467	U
9	A2	470	A
9	A2	486	C
9	A2	487	C
9	A2	489	G
9	A2	490	C
9	A2	491	C
9	A2	492	G
9	A2	498	G
9	A2	500	G
9	A2	501	G
9	A2	502	U
9	A2	504	C
9	A2	505	G
9	A2	510	A
9	A2	511	U
9	A2	513	U
9	A2	514	U
9	A2	515	U
9	A2	673	G
9	A2	674	A
9	A2	675	C
9	A2	681	G
9	A2	692	C
9	A2	693	A
9	A2	694	C
9	A2	703	U
9	A2	704	G
9	A2	711	C
9	A2	715	G

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Mol	Chain	Res	Type
9	A2	735	C
9	A2	736	G
9	A2	738	G
9	A2	740	A
9	A2	746	G
9	A2	747	G
9	A2	748	U
9	A2	749	G
9	A2	750	G
9	A2	751	G
9	A2	753	A
9	A2	756	G
9	A2	767	G
9	A2	770	G
9	A2	801	C
9	A2	802	A
9	A2	803	C
9	A2	809	G
9	A2	812	U
9	A2	814	A
9	A2	816	A
9	A2	822	C
9	A2	824	G
9	A2	831	C
9	A2	834	U
9	A2	839	C
9	A2	841	A
9	A2	842	A
9	A2	843	U
9	A2	844	C
9	A2	855	G
9	A2	857	A
9	A2	858	A
9	A2	859	G
9	A2	869	C
9	A2	877	C
9	A2	878	2MG
9	A2	884	C
9	A2	886	U
9	A2	887	C
9	A2	888	U
9	A2	921	G

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Mol	Chain	Res	Type
9	A2	927	C
9	A2	934	C
9	A2	935	C
9	A2	936	C
9	A2	937	C
9	A2	938	U
9	A2	947	G
9	A2	1000	G
9	A2	1004	C
9	A2	1010	G
9	A2	1011	U
9	A2	1012	C
9	A2	1013	C
9	A2	1014	C
9	A2	1015	C
9	A2	1022	C
9	A2	1024	C
9	A2	1028	G
9	A2	1031	U
9	A2	1032	C
9	A2	1038	G
9	A2	1043	C
9	A2	1044	G
9	A2	1045	G
9	A2	1047	U
9	A2	1049	C
9	A2	1054	G
9	A2	1055	G
9	A2	1060	G
9	A2	1066	C
9	A2	1068	C
9	A2	1070	C
9	A2	1071	G
9	A2	1081	G
9	A2	1082	A
9	A2	1086	C
9	A2	1087	G
9	A2	1089	G
9	A2	1094	C
9	A2	1098	G
9	A2	1099	U
9	A2	1101	G

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Mol	Chain	Res	Type
9	A2	1108	A
9	A2	1110	G
9	A2	1116	U
9	A2	1117	A
9	A2	1118	C
9	A2	1136	A
9	A2	1137	A
9	A2	1140	A2M
9	A2	1158	C
9	A2	1168	A
9	A2	1172	A
9	A2	1173	G
9	A2	1178	U
9	A2	1184	G
9	A2	1191	G
9	A2	1193	C
9	A2	1201	A
9	A2	1207	G
9	A2	1208	G
9	A2	1211	A
9	A2	1212	A
9	A2	1217	C
9	A2	1224	G
9	A2	1229	C
9	A2	1232	G
9	A2	1233	A
9	A2	1252	C
9	A2	1259	C
9	A2	1278	G
9	A2	1298	C
9	A2	1310	A
9	A2	1311	G
9	A2	1315	G
9	A2	1329	G
9	A2	1338	A
9	A2	1347	A2M
9	A2	1360	A
9	A2	1377	A
9	A2	1379	C
9	A2	1388	A
9	A2	1391	U
9	A2	1395	PSU

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Mol	Chain	Res	Type
9	A2	1404	U
9	A2	1409	U
9	A2	1425	G
9	A2	1437	G
9	A2	1438	OMG
9	A2	1439	G
9	A2	1444	A
9	A2	1446	G
9	A2	1447	A
9	A2	1451	A
9	A2	1454	G
9	A2	1455	A
9	A2	1463	A
9	A2	1467	G
9	A2	1473	U
9	A2	1474	C
9	A2	1489	C
9	A2	1490	PSU
9	A2	1504	G
9	A2	1507	C
9	A2	1512	U
9	A2	1522	C
9	A2	1526	G
9	A2	1533	C
9	A2	1538	A
9	A2	1544	A
9	A2	1552	G
9	A2	1558	U
9	A2	1559	U
9	A2	1560	G
9	A2	1564	C
9	A2	1566	G
9	A2	1568	A
9	A2	1569	A
9	A2	1570	C
9	A2	1573	U
9	A2	1589	A
9	A2	1605	G
9	A2	1606	A
9	A2	1607	A
9	A2	1608	G
9	A2	1617	G

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Mol	Chain	Res	Type
9	A2	1621	G
9	A2	1623	G
9	A2	1624	U
9	A2	1625	G
9	A2	1635	G
9	A2	1638	G
9	A2	1639	A
9	A2	1644	G
9	A2	1657	G
9	A2	1665	U
9	A2	1668	UR3
9	A2	1671	G
9	A2	1685	OMG
9	A2	1690	A
9	A2	1699	A
9	A2	1700	C
9	A2	1717	C
9	A2	1721	G
9	A2	1722	C
9	A2	1723	C
9	A2	1724	G
9	A2	1733	C
9	A2	1734	A
9	A2	1737	C
9	A2	1740	C
9	A2	1742	G
9	A2	1750	G
9	A2	1761	U
9	A2	1763	G
9	A2	1766	A
9	A2	1768	C
9	A2	1775	G
9	A2	1776	U
9	A2	1777	G
9	A2	1778	G
9	A2	1779	C
9	A2	1781	A
9	A2	1782	U
9	A2	1783	G
9	A2	1784	G
9	A2	1785	A
9	A2	1786	A

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Mol	Chain	Res	Type
9	A2	1787	G
9	A2	1788	U
9	A2	1789	C
9	A2	1790	G
9	A2	1792	A
9	A2	1793	A
9	A2	1794	U
9	A2	1803	G
9	A2	1804	A
9	A2	1805	G
9	A2	1806	U
9	A2	1807	G
9	A2	1811	A
9	A2	1812	A
9	A2	1813	C
9	A2	1822	U
9	A2	1827	A
9	A2	1828	A
9	A2	1850	U
9	A2	1857	G
9	A2	1858	G
9	A2	1864	C
9	A2	1870	C
9	A2	1871	A
9	A2	1886	C
9	A2	1887	G
9	A2	1893	C
9	A2	1894	G
9	A2	1895	G
9	A2	1897	A
9	A2	1899	G
9	A2	1900	G
9	A2	1903	C
9	A2	1904	G
9	A2	1909	G
9	A2	1910	G
9	A2	1912	A
9	A2	2003	C
9	A2	2004	G
9	A2	2008	G
9	A2	2009	G
9	A2	2012	C

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Mol	Chain	Res	Type
9	A2	2013	C
9	A2	2014	G
9	A2	2015	C
9	A2	2044	C
9	A2	2055	A
9	A2	2056	G
9	A2	2061	G
9	A2	2068	A
9	A2	2071	G
9	A2	2077	G
9	A2	2086	G
9	A2	2088	G
9	A2	2094	G
9	A2	2103	G
9	A2	2106	C
9	A2	2115	A
9	A2	2119	OMG
9	A2	2137	A
9	A2	2150	A
9	A2	2152	G
9	A2	2156	A2M
9	A2	2165	C
9	A2	2172	A
9	A2	2176	G
9	A2	2177	OMC
9	A2	2179	OMG
9	A2	2180	U
9	A2	2181	U
9	A2	2183	A
9	A2	2196	C
9	A2	2229	G
9	A2	2230	G
9	A2	2233	C
9	A2	2239	A
9	A2	2245	U
9	A2	2257	G
9	A2	2258	G
9	A2	2259	C
9	A2	2260	C
9	A2	2262	A
9	A2	2268	A
9	A2	2275	C

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Mol	Chain	Res	Type
9	A2	2284	A
9	A2	2285	U
9	A2	2287	C
9	A2	2299	G
9	A2	2301	G
9	A2	2302	G
9	A2	2321	G
9	A2	2331	G
9	A2	2342	A
9	A2	2344	C
9	A2	2373	G
9	A2	2382	C
9	A2	2383	U
9	A2	2393	G
9	A2	2407	G
9	A2	2411	U
9	A2	2413	G
9	A2	2414	A
9	A2	2416	U
9	A2	2417	G
9	A2	2424	C
9	A2	2430	G
9	A2	2431	A
9	A2	2442	U
9	A2	2449	G
9	A2	2450	A
9	A2	2451	A
9	A2	2458	G
9	A2	2461	G
9	A2	2463	U
9	A2	2466	G
9	A2	2474	C
9	A2	2476	G
9	A2	2478	U
9	A2	2479	G
9	A2	2481	G
9	A2	2494	C
9	A2	2498	A
9	A2	2501	A
9	A2	2507	G
9	A2	2508	G
9	A2	2515	G

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Mol	Chain	Res	Type
9	A2	2516	U
9	A2	2518	U
9	A2	2519	A
9	A2	2524	U
9	A2	2525	C
9	A2	2527	C
9	A2	2528	OMG
9	A2	2543	U
9	A2	2545	U
9	A2	2549	C
9	A2	2554	G
9	A2	2581	U
9	A2	2582	G
9	A2	2590	A
9	A2	2603	G
9	A2	2610	G
9	A2	2611	C
9	A2	2632	G
9	A2	2652	G
9	A2	2659	U
9	A2	3243	C
9	A2	3246	G
9	A2	3250	C
9	A2	3253	G
9	A2	3254	C
9	A2	3271	G
9	A2	3272	U
9	A2	3273	G
9	A2	3282	G
9	A2	3286	A
9	A2	3291	A
9	A2	3302	A
9	A2	3318	A
9	A2	3320	G
9	A2	3329	C
9	A2	3330	G
9	A2	3347	G
9	A2	3348	A
9	A2	3364	C
9	A2	3367	A
9	A2	3368	A
9	A2	3373	A

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Mol	Chain	Res	Type
9	A2	3383	A
9	A2	3385	PSU
9	A2	3392	A
9	A2	3401	U
9	A2	3402	A
9	A2	3404	A
9	A2	3409	G
9	A2	3412	A
9	A2	3415	A
9	A2	3416	A
9	A2	3417	C
9	A2	3420	PSU
9	A2	3422	A
9	A2	3427	C
9	A2	3429	U
9	A2	3430	A
9	A2	3431	A
9	A2	3432	G
9	A2	3433	G
9	A2	3434	U
9	A2	3438	5MC
9	A2	3441	A2M
9	A2	3442	U
9	A2	3458	U
9	A2	3466	C
9	A2	3467	G
9	A2	3470	U
9	A2	3473	A
9	A2	3474	U
9	A2	3475	G
9	A2	3480	A
9	A2	3496	U
9	A2	3499	C
9	A2	3507	U
9	A2	3523	A2M
9	A2	3533	A
9	A2	3534	C
9	A2	3535	G
9	A2	3537	G
9	A2	3543	OMC
9	A2	3546	A
9	A2	3548	U

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Mol	Chain	Res	Type
9	A2	3553	G
9	A2	3554	G
9	A2	3557	A
9	A2	3562	A
9	A2	3563	G
9	A2	3564	A
9	A2	3571	U
9	A2	3582	C
9	A2	3585	G
9	A2	3587	C
9	A2	3594	G
9	A2	3599	A
9	A2	3610	A
9	A2	3612	G
9	A2	3613	U
9	A2	3614	G
9	A2	3615	U
9	A2	3617	G
9	A2	3618	A
9	A2	3619	A
9	A2	3620	U
9	A2	3621	A
9	A2	3622	A
9	A2	3625	G
9	A2	3627	G
9	A2	3630	G
9	A2	3631	C
9	A2	3688	C
9	A2	3689	G
9	A2	3690	C
9	A2	3693	G
9	A2	3694	U
9	A2	3695	G
9	A2	3696	A
9	A2	3697	A
9	A2	3698	A
9	A2	3699	U
9	A2	3701	C
9	A2	3702	C
9	A2	3703	A
9	A2	3704	C
9	A2	3707	C

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Mol	Chain	Res	Type
9	A2	3708	U
9	A2	3712	A
9	A2	3714	C
9	A2	3715	G
9	A2	3726	G
9	A2	3732	G
9	A2	3733	U
9	A2	3734	G
9	A2	3735	A
9	A2	3736	G
9	A2	3742	G
9	A2	3754	G
9	A2	3756	G
9	A2	3757	G
9	A2	3758	G
9	A2	3765	G
9	A2	3766	C
9	A2	3768	U
9	A2	3769	C
9	A2	3771	G
9	A2	3772	G
9	A2	3773	C
9	A2	3777	A
9	A2	3778	A
9	A2	3780	C
9	A2	3782	U
9	A2	3786	U
9	A2	3787	C
9	A2	3792	G
9	A2	3794	G
9	A2	3796	G
9	A2	3814	C
9	A2	3822	A
9	A2	3835	G
9	A2	3836	G
9	A2	3843	G
9	A2	3847	G
9	A2	3853	G
9	A2	3855	A
9	A2	3864	A
9	A2	3873	C
9	A2	3874	G

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Mol	Chain	Res	Type
9	A2	3877	G
9	A2	3881	U
9	A2	3884	U
9	A2	3885	A
9	A2	3886	A
9	A2	3893	C
9	A2	3894	U
9	A2	3895	C
9	A2	3903	A
9	A2	3906	G
9	A2	3907	A
9	A2	3909	A
9	A2	3910	C
9	A2	3917	U
9	A2	3920	A
9	A2	3923	A
9	A2	3925	A
9	A2	3932	A
9	A2	3933	A
9	A2	3941	U
9	A2	3943	G
9	A2	3945	PSU
9	A2	3947	U
9	A2	3956	A
9	A2	3957	G
9	A2	3958	OMU
9	A2	3965	A
9	A2	3966	C
9	A2	3971	C
9	A2	3982	G
9	A2	3984	C
9	A2	3987	5MC
9	A2	4002	C
9	A2	4004	U
9	A2	4006	U
9	A2	4024	U
9	A2	4025	G
9	A2	4029	G
9	A2	4030	A
9	A2	4032	A
9	A2	4033	A
9	A2	4039	C

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Mol	Chain	Res	Type
9	A2	4045	G
9	A2	4046	A
9	A2	4050	C
9	A2	4073	C
9	A2	4096	C
9	A2	4100	G
9	A2	4101	A
9	A2	4102	PSU
9	A2	4104	U
9	A2	4105	C
9	A2	4116	A
9	A2	4118	C
9	A2	4127	G
9	A2	4164	U
9	A2	4165	A
9	A2	4170	A
9	A2	4171	C
9	A2	4174	G
9	A2	4176	G
9	A2	4180	G
9	A2	4183	PSU
9	A2	4184	U
9	A2	4200	A
9	A2	4201	G
9	A2	4212	C
9	A2	4219	G
9	A2	4225	G
9	A2	4227	G
9	A2	4241	A
9	A2	4242	A
9	A2	4252	G
9	A2	4262	A
9	A2	4272	OMU
9	A2	4279	U
9	A2	4287	A
9	A2	4288	PSU
9	A2	4304	G
9	A2	4308	A
9	A2	4310	G
9	A2	4322	C
9	A2	4324	A
9	A2	4331	G

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Mol	Chain	Res	Type
9	A2	4336	A
9	A2	4343	A
9	A2	4347	C
9	A2	4352	A
9	A2	4360	A
9	A2	4361	U
9	A2	4373	G
9	A2	4382	C
9	A2	4383	G
9	A2	4385	C
9	A2	4386	A
9	A2	4392	G
9	A2	4393	A
9	A2	4394	G
9	A2	4402	G
9	A2	4403	G
9	A2	4409	C
9	A2	4411	C
9	A2	4414	A
9	A2	4417	G
9	A2	4422	G
9	A2	4424	U
9	A2	4425	C
9	A2	4429	G
9	A2	4434	U
9	A2	4435	C
9	A2	4436	C
9	A2	4438	C
9	A2	4441	U
9	A2	4491	C
9	A2	4497	U
9	A2	4498	C
9	A2	4499	G
9	A2	4504	C
9	A2	4508	G
9	A2	4509	U
9	A2	4510	C
9	A2	4515	OMG
9	A2	4516	C
9	A2	4519	A
9	A2	4520	G
9	A2	4527	U

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Mol	Chain	Res	Type
9	A2	4528	C
9	A2	4540	C
9	A2	4545	U
9	A2	4546	G
9	A2	4548	G
9	A2	4552	G
9	A2	4553	G
9	A2	4554	A
9	A2	4555	A
9	A2	4557	G
9	A2	4560	G
9	A2	4566	C
9	A2	4569	C
9	A2	4570	U
9	A2	4571	C
9	A2	4573	C
9	A2	4582	U
9	A2	4583	U
9	A2	4587	G
9	A2	4589	A
9	A2	4596	U
9	A2	4609	G
9	A2	4612	A
9	A2	4622	U
9	A2	4634	U
9	A2	4636	C
9	A2	4637	U
9	A2	4652	U
9	A2	4663	G
9	A2	4672	U
9	A2	4680	A
9	A2	4687	G
9	A2	4696	C
9	A2	4701	G
9	A2	4702	A
9	A2	4707	A
9	A2	4715	U
10	B2	7	G
10	B2	11	A
10	B2	22	A
10	B2	24	C
10	B2	33	U

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Mol	Chain	Res	Type
10	B2	47	G
10	B2	50	A
10	B2	53	U
10	B2	54	A
10	B2	63	C
10	B2	64	G
10	B2	89	G
10	B2	93	G
10	B2	100	A
10	B2	110	G
10	B2	120	U
11	C2	14	OMU
11	C2	15	G
11	C2	34	U
11	C2	35	C
11	C2	39	G
11	C2	49	G
11	C2	59	A
11	C2	60	G
11	C2	62	A
11	C2	63	U
11	C2	71	A
11	C2	82	A
11	C2	84	A
11	C2	85	U
11	C2	87	G
11	C2	88	A
11	C2	94	G
11	C2	103	A
11	C2	105	C
11	C2	110	U
11	C2	111	U
11	C2	114	G
11	C2	123	U
11	C2	125	C
11	C2	126	C
11	C2	147	G
11	C2	150	C
11	C2	156	U
46	m2	2	A
46	m2	4	C
46	m2	8	U

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Mol	Chain	Res	Type
46	m2	14	C
46	m2	33	G
46	m2	41	G
46	m2	44	U
46	m2	45	A
46	m2	46	A
46	m2	56	G
46	m2	58	C
46	m2	62	G
46	m2	67	C
46	m2	68	A
46	m2	77	A
46	m2	78	C
46	m2	80	G
46	m2	103	A
46	m2	113	G
46	m2	115	U
46	m2	120	U
46	m2	126	G
46	m2	142	C
46	m2	143	U
46	m2	149	A
46	m2	151	C
46	m2	154	U
46	m2	157	U
46	m2	158	A
46	m2	160	U
46	m2	161	U
46	m2	162	C
46	m2	165	G
46	m2	166	A2M
46	m2	167	G
46	m2	169	U
46	m2	171	A
46	m2	172	U
46	m2	181	A
46	m2	182	C
46	m2	198	U
46	m2	202	C
46	m2	208	G
46	m2	209	G
46	m2	210	G

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Mol	Chain	Res	Type
46	m2	215	G
46	m2	217	G
46	m2	222	U
46	m2	227	G
46	m2	228	A
46	m2	293	G
46	m2	294	A
46	m2	295	C
46	m2	296	U
46	m2	297	C
46	m2	299	A
46	m2	307	U
46	m2	309	G
46	m2	310	G
46	m2	311	G
46	m2	313	C
46	m2	314	G
46	m2	321	C
46	m2	324	C
46	m2	326	C
46	m2	327	C
46	m2	330	U
46	m2	331	G
46	m2	334	G
46	m2	337	G
46	m2	342	C
46	m2	349	G
46	m2	362	A
46	m2	364	C
46	m2	366	A
46	m2	372	G
46	m2	385	G
46	m2	386	U
46	m2	387	G
46	m2	394	A
46	m2	396	G
46	m2	400	A
46	m2	409	G
46	m2	410	A
46	m2	411	C
46	m2	423	G
46	m2	428	A

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Mol	Chain	Res	Type
46	m2	429	U
46	m2	430	U
46	m2	440	G
46	m2	442	G
46	m2	443	C
46	m2	449	A
46	m2	450	A
46	m2	452	C
46	m2	453	G
46	m2	454	G
46	m2	466	A
46	m2	467	A
46	m2	473	G
46	m2	474	C
46	m2	476	G
46	m2	484	G
46	m2	489	U
46	m2	494	C
46	m2	495	A
46	m2	498	C
46	m2	503	C
46	m2	504	C
46	m2	519	OMC
46	m2	524	A
46	m2	531	A
46	m2	533	A
46	m2	536	G
46	m2	539	C
46	m2	544	U
46	m2	546	G
46	m2	551	C
46	m2	556	A
46	m2	557	A
46	m2	559	U
46	m2	562	A
46	m2	565	G
46	m2	566	A
46	m2	570	C
46	m2	585	A
46	m2	587	C
46	m2	589	A
46	m2	591	G

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Mol	Chain	Res	Type
46	m2	593	U
46	m2	595	C
46	m2	598	U
46	m2	602	G
46	m2	606	A
46	m2	609	U
46	m2	619	G
46	m2	624	C
46	m2	625	G
46	m2	629	U
46	m2	630	A
46	m2	645	A
46	m2	657	A
46	m2	662	C
46	m2	670	A2M
46	m2	671	A
46	m2	673	A
46	m2	674	A
46	m2	675	G
46	m2	685	OMG
46	m2	686	G
46	m2	689	C
46	m2	690	U
46	m2	694	G
46	m2	695	A
46	m2	696	G
46	m2	697	C
46	m2	699	G
46	m2	700	G
46	m2	733	G
46	m2	734	U
46	m2	735	C
46	m2	737	C
46	m2	738	C
46	m2	739	G
46	m2	741	C
46	m2	752	C
46	m2	753	G
46	m2	754	G
46	m2	790	G
46	m2	791	G
46	m2	793	C

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Mol	Chain	Res	Type
46	m2	794	C
46	m2	795	G
46	m2	797	A
46	m2	798	G
46	m2	801	U
46	m2	813	A
46	m2	823	G
46	m2	824	PSU
46	m2	832	A
46	m2	836	C
46	m2	838	G
46	m2	839	A
46	m2	841	C
46	m2	844	C
46	m2	849	A
46	m2	863	A
46	m2	864	A
46	m2	871	A
46	m2	872	A
46	m2	875	G
46	m2	876	G
46	m2	877	A
46	m2	878	C
46	m2	885	U
46	m2	886	C
46	m2	889	U
46	m2	890	U
46	m2	895	U
46	m2	896	G
46	m2	897	G
46	m2	898	U
46	m2	899	U
46	m2	901	U
46	m2	915	A
46	m2	919	U
46	m2	922	A
46	m2	924	A
46	m2	935	G
46	m2	936	G
46	m2	952	C
46	m2	971	U
46	m2	973	G

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Mol	Chain	Res	Type
46	m2	980	G
46	m2	990	C
46	m2	992	A
46	m2	994	A
46	m2	999	A
46	m2	1001	G
46	m2	1003	A
46	m2	1019	U
46	m2	1025	A
46	m2	1029	A
46	m2	1047	U
46	m2	1063	U
46	m2	1064	A
46	m2	1085	A
46	m2	1087	C
46	m2	1117	U
46	m2	1118	C
46	m2	1120	C
46	m2	1123	G
46	m2	1133	G
46	m2	1135	A
46	m2	1140	C
46	m2	1152	A
46	m2	1155	C
46	m2	1156	U
46	m2	1172	A
46	m2	1197	A
46	m2	1217	C
46	m2	1218	C
46	m2	1219	A
46	m2	1226	G
46	m2	1229	G
46	m2	1230	A
46	m2	1242	A
46	m2	1243	A
46	m2	1244	U
46	m2	1245	PSU
46	m2	1251	C
46	m2	1253	A
46	m2	1255	A
46	m2	1258	G
46	m2	1259	G

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Mol	Chain	Res	Type
46	m2	1274	C
46	m2	1275	C
46	m2	1276	G
46	m2	1277	G
46	m2	1285	C
46	m2	1288	G
46	m2	1299	U
46	m2	1300	G
46	m2	1302	U
46	m2	1304	G
46	m2	1305	C
46	m2	1310	U
46	m2	1315	A
46	m2	1335	U
46	m2	1343	C
46	m2	1344	U
46	m2	1345	U
46	m2	1346	A
46	m2	1356	G
46	m2	1373	U
46	m2	1374	U
46	m2	1377	G
46	m2	1380	A
46	m2	1384	A
46	m2	1398	A
46	m2	1399	U
46	m2	1400	G
46	m2	1404	A
46	m2	1414	C
46	m2	1417	C
46	m2	1419	C
46	m2	1420	C
46	m2	1421	C
46	m2	1422	G
46	m2	1424	G
46	m2	1426	G
46	m2	1431	G
46	m2	1435	C
46	m2	1436	C
46	m2	1437	C
46	m2	1438	C
46	m2	1439	C

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Mol	Chain	Res	Type
46	m2	1440	A
46	m2	1444	U
46	m2	1446	U
46	m2	1448	A
46	m2	1452	G
46	m2	1454	A
46	m2	1455	C
46	m2	1456	A
46	m2	1465	U
46	m2	1473	C
46	m2	1475	G
46	m2	1490	C
46	m2	1491	A
46	m2	1492	G
46	m2	1496	U
46	m2	1499	G
46	m2	1500	A
46	m2	1507	U
46	m2	1509	G
46	m2	1510	A
46	m2	1520	C
46	m2	1522	G
46	m2	1523	C
46	m2	1533	A
46	m2	1535	A
46	m2	1554	G
46	m2	1555	C
46	m2	1557	U
46	m2	1558	A
46	m2	1560	C
46	m2	1562	U
46	m2	1570	C
46	m2	1577	G
46	m2	1582	A
46	m2	1587	U
46	m2	1589	G
46	m2	1590	A
46	m2	1594	C
46	m2	1603	A
46	m2	1606	G
46	m2	1608	G
46	m2	1619	G

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Mol	Chain	Res	Type
46	m2	1623	U
46	m2	1625	A
46	m2	1626	U
46	m2	1632	A
46	m2	1636	A
46	m2	1638	G
46	m2	1639	A
46	m2	1640	G
46	m2	1650	G
46	m2	1656	G
46	m2	1662	C
46	m2	1665	A
46	m2	1667	G
46	m2	1680	A
46	m2	1682	G
46	m2	1685	C
46	m2	1703	C
46	m2	1711	G
46	m2	1714	A
46	m2	1717	A
46	m2	1723	U
46	m2	1724	G
46	m2	1731	U
46	m2	1747	A
46	m2	1753	C
46	m2	1756	G
46	m2	1759	G
46	m2	1777	U
46	m2	1784	G
46	m2	1785	C
46	m2	1786	G
46	m2	1815	A
46	m2	1827	A
46	m2	1832	UR3
46	m2	1833	A
46	m2	1837	A
46	m2	1840	U
46	m2	1851	G
46	m2	1853	A
46	m2	1854	C
46	m2	1863	G
46	m2	1864	G

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Mol	Chain	Res	Type
46	m2	1865	A
46	m2	1867	C
46	m2	1868	A
46	m2	1869	U
47	n2	9	U
47	n2	10	G
47	n2	11	G
47	n2	13	G
47	n2	15	A
47	n2	16	G
47	n2	17	C
47	n2	18	G
47	n2	19	G
47	n2	21	A
47	n2	26	G
47	n2	31	G
47	n2	34	C
47	n2	35	A
47	n2	37	A
47	n2	47	U
47	n2	48	C
47	n2	57	G
47	n2	58	A
47	n2	61	C
47	n2	63	A
47	n2	67	U
47	n2	75	C
47	n2	76	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A2	143	U
9	A2	406	C
9	A2	1438	OMG
9	A2	1446	G
9	A2	1778	G
9	A2	1787	G
9	A2	1792	A
9	A2	2382	C
9	A2	2430	G
9	A2	3772	G

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Mol	Chain	Res	Type
9	A2	4330	G
9	A2	4351	U
9	A2	4582	U
11	C2	59	A
11	C2	83	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	OMU	m2	116	46	19,22,23	3.00	8 (42%)	26,31,34	1.61	4 (15%)
9	B8T	A2	4135	9	19,22,23	3.26	8 (42%)	26,31,34	0.85	1 (3%)
9	UR3	A2	1668	9	19,22,23	3.19	7 (36%)	26,32,35	1.35	3 (11%)
9	6MZ	A2	3872	9	18,25,26	1.83	3 (16%)	16,36,39	1.86	2 (12%)
9	UR3	A2	4249	9	19,22,23	3.14	7 (36%)	26,32,35	1.27	3 (11%)
46	PSU	m2	614	46	18,21,22	4.33	6 (33%)	22,30,33	2.70	6 (27%)
9	A2M	A2	3523	9	18,25,26	2.67	10 (55%)	18,36,39	1.85	4 (22%)
9	PSU	A2	3385	9	18,21,22	4.35	6 (33%)	22,30,33	2.76	5 (22%)
9	B8W	A2	3837	9	18,26,27	6.03	9 (50%)	21,38,41	3.31	9 (42%)
9	5MC	A2	4099	9	18,22,23	3.56	7 (38%)	26,32,35	1.03	1 (3%)
9	OMU	A2	4272	9	19,22,23	3.00	8 (42%)	26,31,34	1.66	4 (15%)
9	PSU	A2	4280	9	18,21,22	4.37	6 (33%)	22,30,33	2.74	5 (22%)
9	A2M	A2	3379	9	18,25,26	2.63	9 (50%)	18,36,39	1.87	4 (22%)
9	PSU	A2	3420	9	18,21,22	4.35	6 (33%)	22,30,33	2.63	5 (22%)
9	G7M	A2	2277	9	20,26,27	3.97	9 (45%)	17,39,42	1.12	1 (5%)
9	A2M	A2	4223	9	18,25,26	2.64	9 (50%)	18,36,39	1.89	4 (22%)
9	OMC	A2	3357	9	19,22,23	3.02	8 (42%)	26,31,34	0.71	0
9	A2M	A2	3481	9	18,25,26	2.64	9 (50%)	18,36,39	1.89	4 (22%)
46	A2M	m2	1033	46	18,25,26	2.64	9 (50%)	18,36,39	1.84	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	A2M	m2	27	46	18,25,26	2.65	10 (55%)	18,36,39	1.82	3 (16%)
46	UR3	m2	1832	46	19,22,23	3.15	7 (36%)	26,32,35	1.32	2 (7%)
9	PSU	A2	4183	9	18,21,22	4.37	6 (33%)	22,30,33	2.84	5 (22%)
9	OMU	A2	3958	9	19,22,23	2.98	8 (42%)	26,31,34	1.71	5 (19%)
46	PSU	m2	824	46	18,21,22	4.37	6 (33%)	22,30,33	2.72	5 (22%)
9	A2M	A2	1337	9	18,25,26	2.63	9 (50%)	18,36,39	1.83	4 (22%)
9	A2M	A2	1347	9	18,25,26	2.73	10 (55%)	18,36,39	1.92	4 (22%)
9	E7G	A2	1599	9	24,27,28	3.74	10 (41%)	30,40,43	2.23	10 (33%)
9	PSU	A2	4102	9	18,21,22	4.34	6 (33%)	22,30,33	2.73	5 (22%)
46	PSU	m2	1245	46	18,21,22	4.38	6 (33%)	22,30,33	2.71	5 (22%)
46	PSU	m2	1083	46	18,21,22	4.35	6 (33%)	22,30,33	2.76	5 (22%)
9	OMC	A2	4188	9	19,22,23	3.01	8 (42%)	26,31,34	0.79	0
9	OMG	A2	1852	9	18,26,27	2.58	8 (44%)	19,38,41	1.49	4 (21%)
9	A2M	A2	1140	9	18,25,26	2.67	10 (55%)	18,36,39	1.92	4 (22%)
9	OMG	A2	2528	9	18,26,27	2.61	8 (44%)	19,38,41	1.52	4 (21%)
9	PSU	A2	1395	9	18,21,22	4.37	7 (38%)	22,30,33	2.69	5 (22%)
9	PSU	A2	4152	9	18,21,22	4.39	7 (38%)	22,30,33	2.81	5 (22%)
9	I4U	A2	3846	9	21,24,25	4.74	16 (76%)	27,34,37	1.08	1 (3%)
46	4AC	m2	1844	46	21,24,25	3.67	9 (42%)	29,34,37	1.10	3 (10%)
9	MHG	A2	4023	9	29,32,33	4.05	10 (34%)	34,46,49	2.55	12 (35%)
14	MLZ	F2	333	14	8,9,10	0.71	0	4,9,11	0.92	0
9	PSU	A2	4094	9	18,21,22	4.41	7 (38%)	22,30,33	2.75	6 (27%)
9	A2M	A2	2118	9	18,25,26	2.64	10 (55%)	18,36,39	1.81	4 (22%)
46	A2M	m2	670	46	18,25,26	2.69	10 (55%)	18,36,39	1.82	4 (22%)
9	OMG	A2	4275	9	18,26,27	2.60	8 (44%)	19,38,41	1.53	4 (21%)
9	E6G	A2	4007	9	20,27,28	5.76	8 (40%)	22,39,42	2.06	6 (27%)
9	OMC	A2	3565	9	19,22,23	3.05	8 (42%)	26,31,34	0.81	0
9	B9B	A2	237	9	21,28,29	5.60	8 (38%)	23,40,43	1.97	5 (21%)
9	OMG	A2	4022	43,9	18,26,27	2.59	8 (44%)	19,38,41	1.50	4 (21%)
9	2MG	A2	4517	9,7	18,26,27	2.14	6 (33%)	16,38,41	1.40	4 (25%)
9	PSU	A2	1496	9	18,21,22	4.34	6 (33%)	22,30,33	2.79	5 (22%)
9	B9H	A2	2541	9	20,25,26	2.93	5 (25%)	22,35,38	1.63	4 (18%)
9	OMC	A2	2177	9	19,22,23	3.03	8 (42%)	26,31,34	0.96	1 (3%)
9	A2M	A2	1673	9	18,25,26	2.62	9 (50%)	18,36,39	1.92	4 (22%)
46	B8N	m2	1250	46	24,29,30	2.47	5 (20%)	29,42,45	1.84	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	B9B	A2	1387	9	21,28,29	5.62	8 (38%)	23,40,43	1.91	6 (26%)
46	OMG	m2	646	46	18,26,27	2.61	8 (44%)	19,38,41	1.49	4 (21%)
9	I4U	A2	1472	9	21,24,25	4.74	16 (76%)	27,34,37	1.16	2 (7%)
9	OMG	A2	4146	9	18,26,27	2.60	8 (44%)	19,38,41	1.50	4 (21%)
11	OMU	C2	14	11	19,22,23	3.04	8 (42%)	26,31,34	1.70	4 (15%)
9	1MA	A2	4067	9	16,25,26	3.96	3 (18%)	18,37,40	1.67	3 (16%)
9	OMG	A2	1438	9	18,26,27	2.59	8 (44%)	19,38,41	1.56	4 (21%)
9	G7M	A2	1418	9	20,26,27	3.97	9 (45%)	17,39,42	1.14	1 (5%)
9	2MG	A2	1330	9	18,26,27	2.17	6 (33%)	16,38,41	1.39	4 (25%)
9	OMG	A2	4289	9,32	18,26,27	2.59	7 (38%)	19,38,41	1.49	3 (15%)
9	OMG	A2	2119	9	18,26,27	2.58	8 (44%)	19,38,41	1.53	4 (21%)
9	PSU	A2	3371	9	18,21,22	4.34	6 (33%)	22,30,33	2.69	6 (27%)
46	PSU	m2	825	46	18,21,22	4.37	7 (38%)	22,30,33	2.78	5 (22%)
9	OMG	A2	1685	9,33	18,26,27	2.60	8 (44%)	19,38,41	1.55	4 (21%)
9	OMC	A2	2120	9	19,22,23	3.02	7 (36%)	26,31,34	1.02	3 (11%)
9	5MC	A2	3438	9	18,22,23	3.61	7 (38%)	26,32,35	0.98	1 (3%)
9	OMG	A2	3448	9	18,26,27	2.59	8 (44%)	19,38,41	1.50	4 (21%)
9	A2M	A2	3374	9	18,25,26	2.64	9 (50%)	18,36,39	1.86	4 (22%)
9	A2M	A2	3441	9	18,25,26	2.77	9 (50%)	18,36,39	1.85	3 (16%)
9	B8Q	A2	1269	9	17,22,23	3.10	4 (23%)	22,32,35	1.98	6 (27%)
9	E7G	A2	2052	9	24,27,28	3.72	10 (41%)	30,40,43	2.22	9 (30%)
9	OMC	A2	3543	9,17	19,22,23	3.03	8 (42%)	26,31,34	0.84	0
9	OMG	A2	3848	9	18,26,27	2.60	8 (44%)	19,38,41	1.50	4 (21%)
9	G7M	A2	4202	9	20,26,27	3.97	9 (45%)	17,39,42	1.12	1 (5%)
79	DDE	m	714	79	14,20,21	2.00	3 (21%)	14,28,30	1.53	2 (14%)
9	A2M	A2	398	9	18,25,26	2.63	9 (50%)	18,36,39	1.89	4 (22%)
9	PSU	A2	2263	9	18,21,22	4.38	6 (33%)	22,30,33	2.67	5 (22%)
9	OMG	A2	1335	9	18,26,27	2.60	8 (44%)	19,38,41	1.56	4 (21%)
9	OMG	A2	4515	9,7	18,26,27	2.58	8 (44%)	19,38,41	1.53	4 (21%)
9	PSU	A2	4055	9	18,21,22	4.36	6 (33%)	22,30,33	2.76	6 (27%)
9	P7G	A2	3536	9	24,28,29	4.01	10 (41%)	27,41,44	1.52	2 (7%)
41	MLZ	g2	98	41	8,9,10	0.70	0	4,9,11	0.90	0
9	PSU	A2	4288	9,32	18,21,22	4.36	7 (38%)	22,30,33	2.74	5 (22%)
9	OMG	A2	373	9	18,26,27	2.59	8 (44%)	19,38,41	1.51	4 (21%)
9	OMG	A2	2179	9	18,26,27	2.61	8 (44%)	19,38,41	1.50	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	OMG	m2	685	46	18,26,27	2.60	8 (44%)	19,38,41	1.49	4 (21%)
9	OMC	A2	3525	9	19,22,23	3.01	8 (42%)	26,31,34	0.74	0
46	OMC	m2	519	46	19,22,23	3.05	8 (42%)	26,31,34	0.90	1 (3%)
9	OMC	A2	2559	9	19,22,23	3.01	8 (42%)	26,31,34	0.73	0
9	5MC	A2	3987	9	18,22,23	3.59	7 (38%)	26,32,35	1.04	2 (7%)
9	PSU	A2	1490	9	18,21,22	4.36	6 (33%)	22,30,33	2.78	6 (27%)
46	A2M	m2	166	46	18,25,26	2.65	9 (50%)	18,36,39	1.93	4 (22%)
9	2MG	A2	878	9	18,26,27	2.16	6 (33%)	16,38,41	1.34	3 (18%)
9	OMC	A2	2616	9	19,22,23	3.07	8 (42%)	26,31,34	0.90	1 (3%)
9	P7G	A2	1711	9,10	24,28,29	4.09	10 (41%)	27,41,44	1.44	2 (7%)
9	PSU	A2	3945	9	18,21,22	4.32	6 (33%)	22,30,33	2.77	5 (22%)
9	A2M	A2	2156	9	18,25,26	2.66	9 (50%)	18,36,39	1.85	4 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	OMU	m2	116	46	-	1/9/27/28	0/2/2/2
9	B8T	A2	4135	9	-	0/7/27/28	0/2/2/2
9	UR3	A2	1668	9	-	2/7/25/26	0/2/2/2
9	6MZ	A2	3872	9	-	5/5/27/28	0/3/3/3
9	UR3	A2	4249	9	-	0/7/25/26	0/2/2/2
46	PSU	m2	614	46	-	0/7/25/26	0/2/2/2
9	A2M	A2	3523	9	-	3/5/27/28	0/3/3/3
9	PSU	A2	3385	9	-	2/7/25/26	0/2/2/2
9	B8W	A2	3837	9	-	2/5/27/28	0/3/3/3
9	5MC	A2	4099	9	-	4/7/25/26	0/2/2/2
9	OMU	A2	4272	9	-	1/9/27/28	0/2/2/2
9	PSU	A2	4280	9	-	0/7/25/26	0/2/2/2
9	A2M	A2	3379	9	-	1/5/27/28	0/3/3/3
9	PSU	A2	3420	9	-	2/7/25/26	0/2/2/2
9	G7M	A2	2277	9	-	0/3/25/26	0/3/3/3
9	A2M	A2	4223	9	-	1/5/27/28	0/3/3/3
9	OMC	A2	3357	9	-	5/9/27/28	0/2/2/2
9	A2M	A2	3481	9	-	1/5/27/28	0/3/3/3
46	A2M	m2	1033	46	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	A2M	m2	27	46	-	1/5/27/28	0/3/3/3
46	UR3	m2	1832	46	-	4/7/25/26	0/2/2/2
9	PSU	A2	4183	9	-	1/7/25/26	0/2/2/2
9	OMU	A2	3958	9	-	3/9/27/28	0/2/2/2
46	PSU	m2	824	46	-	3/7/25/26	0/2/2/2
9	A2M	A2	1337	9	-	0/5/27/28	0/3/3/3
9	A2M	A2	1347	9	-	2/5/27/28	0/3/3/3
9	E7G	A2	1599	9	-	1/9/39/40	0/3/3/3
9	PSU	A2	4102	9	-	3/7/25/26	0/2/2/2
46	PSU	m2	1245	46	-	3/7/25/26	0/2/2/2
46	PSU	m2	1083	46	-	1/7/25/26	0/2/2/2
9	OMC	A2	4188	9	-	0/9/27/28	0/2/2/2
9	OMG	A2	1852	9	-	0/5/27/28	0/3/3/3
9	A2M	A2	1140	9	-	1/5/27/28	0/3/3/3
9	OMG	A2	2528	9	-	2/5/27/28	0/3/3/3
9	PSU	A2	1395	9	-	2/7/25/26	0/2/2/2
9	PSU	A2	4152	9	-	4/7/25/26	0/2/2/2
9	I4U	A2	3846	9	-	2/9/29/30	0/2/2/2
46	4AC	m2	1844	46	-	0/11/29/30	0/2/2/2
9	MHG	A2	4023	9	-	4/16/46/47	0/3/3/3
14	MLZ	F2	333	14	-	1/7/8/10	-
9	PSU	A2	4094	9	-	0/7/25/26	0/2/2/2
9	A2M	A2	2118	9	-	0/5/27/28	0/3/3/3
46	A2M	m2	670	46	-	1/5/27/28	0/3/3/3
9	OMG	A2	4275	9	-	0/5/27/28	0/3/3/3
9	E6G	A2	4007	9	-	3/6/28/29	0/3/3/3
9	OMC	A2	3565	9	-	0/9/27/28	0/2/2/2
9	B9B	A2	237	9	-	6/7/29/30	0/3/3/3
9	OMG	A2	4022	43,9	-	0/5/27/28	0/3/3/3
9	2MG	A2	4517	9,7	-	0/5/27/28	0/3/3/3
9	PSU	A2	1496	9	-	0/7/25/26	0/2/2/2
9	B9H	A2	2541	9	-	0/12/47/48	0/2/2/2
9	OMC	A2	2177	9	-	5/9/27/28	0/2/2/2
9	A2M	A2	1673	9	-	0/5/27/28	0/3/3/3
46	B8N	m2	1250	46	-	4/16/34/35	0/2/2/2
9	B9B	A2	1387	9	-	3/7/29/30	0/3/3/3
46	OMG	m2	646	46	-	2/5/27/28	0/3/3/3
9	I4U	A2	1472	9	-	0/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	OMG	A2	4146	9	-	0/5/27/28	0/3/3/3
11	OMU	C2	14	11	-	1/9/27/28	0/2/2/2
9	1MA	A2	4067	9	-	2/3/25/26	0/3/3/3
9	OMG	A2	1438	9	-	3/5/27/28	0/3/3/3
9	G7M	A2	1418	9	-	0/3/25/26	0/3/3/3
9	2MG	A2	1330	9	-	0/5/27/28	0/3/3/3
9	OMG	A2	4289	9,32	-	2/5/27/28	0/3/3/3
9	OMG	A2	2119	9	-	2/5/27/28	0/3/3/3
9	PSU	A2	3371	9	-	0/7/25/26	0/2/2/2
46	PSU	m2	825	46	-	0/7/25/26	0/2/2/2
9	OMG	A2	1685	9,33	-	2/5/27/28	0/3/3/3
9	OMC	A2	2120	9	-	0/9/27/28	0/2/2/2
9	5MC	A2	3438	9	-	2/7/25/26	0/2/2/2
9	OMG	A2	3448	9	-	0/5/27/28	0/3/3/3
9	A2M	A2	3374	9	-	1/5/27/28	0/3/3/3
9	A2M	A2	3441	9	-	2/5/27/28	0/3/3/3
9	B8Q	A2	1269	9	-	0/7/42/43	0/2/2/2
9	E7G	A2	2052	9	-	4/9/39/40	0/3/3/3
9	OMC	A2	3543	9,17	-	3/9/27/28	0/2/2/2
9	OMG	A2	3848	9	-	0/5/27/28	0/3/3/3
9	G7M	A2	4202	9	-	0/3/25/26	0/3/3/3
79	DDE	m	714	79	-	7/20/21/23	0/1/1/1
9	A2M	A2	398	9	-	3/5/27/28	0/3/3/3
9	PSU	A2	2263	9	-	0/7/25/26	0/2/2/2
9	OMG	A2	1335	9	-	0/5/27/28	0/3/3/3
9	OMG	A2	4515	9,7	-	1/5/27/28	0/3/3/3
9	PSU	A2	4055	9	-	0/7/25/26	0/2/2/2
9	P7G	A2	3536	9	-	3/10/40/41	0/3/3/3
41	MLZ	g2	98	41	-	1/7/8/10	-
9	PSU	A2	4288	9,32	-	6/7/25/26	0/2/2/2
9	OMG	A2	373	9	-	1/5/27/28	0/3/3/3
9	OMG	A2	2179	9	-	3/5/27/28	0/3/3/3
46	OMG	m2	685	46	-	2/5/27/28	0/3/3/3
9	OMC	A2	3525	9	-	0/9/27/28	0/2/2/2
46	OMC	m2	519	46	-	4/9/27/28	0/2/2/2
9	OMC	A2	2559	9	-	0/9/27/28	0/2/2/2
9	5MC	A2	3987	9	-	1/7/25/26	0/2/2/2
9	PSU	A2	1490	9	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	A2M	m2	166	46	-	3/5/27/28	0/3/3/3
9	2MG	A2	878	9	-	2/5/27/28	0/3/3/3
9	OMC	A2	2616	9	-	0/9/27/28	0/2/2/2
9	P7G	A2	1711	9,10	-	1/10/40/41	0/3/3/3
9	PSU	A2	3945	9	-	2/7/25/26	0/2/2/2
9	A2M	A2	2156	9	-	2/5/27/28	0/3/3/3

All (772) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3837	B8W	O4'-C1'	19.05	1.67	1.41
9	A2	1387	B9B	C2'-C1'	-15.85	1.29	1.53
9	A2	4007	E6G	O4'-C1'	15.81	1.63	1.41
9	A2	237	B9B	O4'-C1'	15.69	1.63	1.41
9	A2	4007	E6G	C2'-C1'	-15.65	1.30	1.53
9	A2	1387	B9B	O4'-C1'	15.54	1.62	1.41
9	A2	237	B9B	C2'-C1'	-15.53	1.30	1.53
9	A2	4067	1MA	C2-N3	14.82	1.47	1.29
9	A2	3837	B8W	C2'-C1'	-12.98	1.34	1.53
46	m2	1245	PSU	C6-C5	12.07	1.49	1.35
9	A2	4094	PSU	C6-C5	12.00	1.49	1.35
9	A2	2263	PSU	C6-C5	11.99	1.49	1.35
9	A2	4183	PSU	C6-C5	11.95	1.49	1.35
9	A2	4152	PSU	C6-C5	11.95	1.49	1.35
9	A2	4280	PSU	C6-C5	11.95	1.49	1.35
9	A2	1395	PSU	C6-C5	11.90	1.49	1.35
9	A2	3420	PSU	C6-C5	11.90	1.49	1.35
9	A2	4055	PSU	C6-C5	11.88	1.49	1.35
46	m2	825	PSU	C6-C5	11.87	1.49	1.35
46	m2	1083	PSU	C6-C5	11.84	1.49	1.35
9	A2	1496	PSU	C6-C5	11.84	1.49	1.35
46	m2	824	PSU	C6-C5	11.84	1.49	1.35
9	A2	4288	PSU	C6-C5	11.83	1.49	1.35
9	A2	3371	PSU	C6-C5	11.82	1.49	1.35
9	A2	3385	PSU	C6-C5	11.81	1.49	1.35
46	m2	614	PSU	C6-C5	11.73	1.49	1.35
9	A2	4023	MHG	C8-N9	11.73	1.52	1.46
9	A2	4102	PSU	C6-C5	11.72	1.49	1.35
9	A2	3945	PSU	C6-C5	11.70	1.48	1.35
9	A2	1490	PSU	C6-C5	11.69	1.48	1.35
9	A2	1472	I4U	C4-N3	10.81	1.45	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3846	I4U	C4-N3	10.72	1.45	1.31
9	A2	1711	P7G	C8-N9	10.49	1.51	1.46
9	A2	3536	P7G	C8-N9	10.34	1.51	1.46
9	A2	4202	G7M	C8-N7	10.13	1.51	1.33
9	A2	1418	G7M	C8-N7	10.10	1.51	1.33
9	A2	2277	G7M	C8-N7	10.10	1.51	1.33
9	A2	2277	G7M	C8-N9	9.96	1.51	1.33
9	A2	1418	G7M	C8-N9	9.93	1.51	1.33
9	A2	1472	I4U	C3'-C2'	-9.93	1.26	1.53
9	A2	4202	G7M	C8-N9	9.92	1.51	1.33
9	A2	3846	I4U	C3'-C2'	-9.87	1.26	1.53
9	A2	2052	E7G	C8-N9	9.74	1.51	1.46
9	A2	1490	PSU	C2-N1	9.62	1.49	1.36
9	A2	2263	PSU	C2-N1	9.60	1.49	1.36
9	A2	4152	PSU	C2-N1	9.59	1.49	1.36
9	A2	4102	PSU	C2-N1	9.59	1.49	1.36
46	m2	825	PSU	C2-N1	9.58	1.49	1.36
9	A2	1599	E7G	C8-N9	9.57	1.51	1.46
46	m2	1083	PSU	C2-N1	9.54	1.49	1.36
9	A2	3385	PSU	C2-N1	9.54	1.49	1.36
9	A2	1395	PSU	C2-N1	9.53	1.49	1.36
9	A2	4055	PSU	C2-N1	9.52	1.49	1.36
9	A2	4288	PSU	C2-N1	9.52	1.49	1.36
9	A2	4183	PSU	C2-N1	9.52	1.49	1.36
9	A2	3945	PSU	C2-N1	9.51	1.49	1.36
9	A2	4280	PSU	C2-N1	9.49	1.49	1.36
9	A2	1496	PSU	C2-N1	9.48	1.49	1.36
46	m2	1245	PSU	C2-N1	9.47	1.49	1.36
9	A2	4094	PSU	C2-N1	9.44	1.49	1.36
46	m2	824	PSU	C2-N1	9.42	1.49	1.36
9	A2	3371	PSU	C2-N1	9.40	1.49	1.36
46	m2	614	PSU	C2-N1	9.37	1.49	1.36
9	A2	3420	PSU	C2-N1	9.35	1.49	1.36
9	A2	3438	5MC	C6-C5	9.32	1.49	1.34
9	A2	3987	5MC	C6-C5	9.23	1.49	1.34
9	A2	1711	P7G	C5-N7	9.17	1.45	1.35
9	A2	1668	UR3	C2-N1	9.14	1.51	1.38
9	A2	4099	5MC	C6-C5	9.09	1.49	1.34
9	A2	4023	MHG	C5-N7	9.05	1.45	1.35
9	A2	4249	UR3	C2-N1	8.85	1.51	1.38
46	m2	1832	UR3	C2-N1	8.79	1.51	1.38
9	A2	4023	MHG	C2-N3	8.78	1.48	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3536	P7G	C5-N7	8.62	1.45	1.35
9	A2	2541	B9H	C2-N3	8.44	1.48	1.37
9	A2	1269	B8Q	C2-N3	8.34	1.49	1.35
9	A2	1599	E7G	C5-N7	8.20	1.44	1.35
9	A2	2052	E7G	C5-N7	8.03	1.44	1.35
46	m2	1844	4AC	C4-N3	7.94	1.46	1.32
9	A2	4007	E6G	O4'-C4'	-7.64	1.27	1.45
9	A2	1387	B9B	O4'-C4'	-7.63	1.27	1.45
9	A2	237	B9B	O4'-C4'	-7.52	1.28	1.45
46	m2	824	PSU	C2-N3	7.48	1.50	1.37
9	A2	4023	MHG	C4-N9	7.27	1.46	1.37
9	A2	3441	A2M	O4'-C1'	-7.26	1.30	1.41
9	A2	4102	PSU	C2-N3	7.24	1.49	1.37
9	A2	4094	PSU	C2-N3	7.23	1.49	1.37
9	A2	4152	PSU	C2-N3	7.23	1.49	1.37
46	m2	825	PSU	C2-N3	7.22	1.49	1.37
9	A2	4280	PSU	C2-N3	7.22	1.49	1.37
9	A2	4183	PSU	C2-N3	7.21	1.49	1.37
9	A2	1395	PSU	C2-N3	7.21	1.49	1.37
9	A2	4288	PSU	C2-N3	7.20	1.49	1.37
9	A2	1490	PSU	C2-N3	7.19	1.49	1.37
46	m2	614	PSU	C2-N3	7.18	1.49	1.37
9	A2	3371	PSU	C2-N3	7.18	1.49	1.37
46	m2	1245	PSU	C2-N3	7.17	1.49	1.37
9	A2	4135	B8T	C4-N3	7.16	1.45	1.32
9	A2	1496	PSU	C2-N3	7.15	1.49	1.37
9	A2	3385	PSU	C2-N3	7.15	1.49	1.37
9	A2	3945	PSU	C2-N3	7.15	1.49	1.37
46	m2	1844	4AC	C2-N3	7.11	1.50	1.36
9	A2	4055	PSU	C2-N3	7.10	1.49	1.37
9	A2	3420	PSU	C2-N3	7.10	1.49	1.37
46	m2	1083	PSU	C2-N3	7.09	1.49	1.37
9	A2	4023	MHG	C8-N7	7.06	1.52	1.45
9	A2	2263	PSU	C2-N3	7.06	1.49	1.37
46	m2	1250	B8N	C4-N3	-7.02	1.27	1.40
9	A2	1347	A2M	O4'-C1'	-7.01	1.31	1.41
11	C2	14	OMU	C2-N1	7.00	1.49	1.38
9	A2	1711	P7G	C8-N7	6.94	1.52	1.45
9	A2	4272	OMU	C2-N3	6.93	1.50	1.38
46	m2	116	OMU	C2-N3	6.90	1.50	1.38
9	A2	1269	B8Q	C6-C5	6.90	1.48	1.33
46	m2	1844	4AC	C6-C5	6.88	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	m2	116	OMU	C2-N1	6.87	1.49	1.38
9	A2	4272	OMU	C2-N1	6.86	1.49	1.38
9	A2	2541	B9H	C6-C5	6.83	1.48	1.33
46	m2	670	A2M	O4'-C1'	-6.81	1.31	1.41
11	C2	14	OMU	C2-N3	6.80	1.50	1.38
9	A2	3958	OMU	C2-N3	6.80	1.50	1.38
9	A2	3837	B8W	O4'-C4'	-6.71	1.30	1.45
9	A2	3958	OMU	C2-N1	6.71	1.49	1.38
9	A2	1140	A2M	O4'-C1'	-6.62	1.31	1.41
9	A2	3536	P7G	C4-N9	6.62	1.45	1.35
9	A2	3438	5MC	C4-N3	6.56	1.45	1.34
9	A2	3523	A2M	O4'-C1'	-6.55	1.31	1.41
9	A2	1711	P7G	C4-N9	6.53	1.44	1.35
9	A2	3987	5MC	C4-N3	6.53	1.45	1.34
9	A2	2156	A2M	O4'-C1'	-6.52	1.32	1.41
9	A2	2616	OMC	C2-N3	6.49	1.49	1.36
9	A2	3872	6MZ	C6-N6	6.48	1.45	1.35
9	A2	4099	5MC	C4-N3	6.47	1.45	1.34
9	A2	1337	A2M	O4'-C1'	-6.47	1.32	1.41
9	A2	3565	OMC	C2-N3	6.47	1.49	1.36
9	A2	2120	OMC	C2-N3	6.46	1.49	1.36
46	m2	27	A2M	O4'-C1'	-6.43	1.32	1.41
9	A2	3481	A2M	O4'-C1'	-6.43	1.32	1.41
9	A2	2118	A2M	O4'-C1'	-6.43	1.32	1.41
9	A2	4223	A2M	O4'-C1'	-6.43	1.32	1.41
46	m2	166	A2M	O4'-C1'	-6.42	1.32	1.41
9	A2	3357	OMC	C2-N3	6.40	1.49	1.36
9	A2	2177	OMC	C2-N3	6.40	1.49	1.36
9	A2	2559	OMC	C2-N3	6.39	1.49	1.36
46	m2	1844	4AC	C4-N4	6.39	1.49	1.39
9	A2	3379	A2M	O4'-C1'	-6.38	1.32	1.41
46	m2	1033	A2M	O4'-C1'	-6.38	1.32	1.41
46	m2	519	OMC	C2-N3	6.36	1.49	1.36
9	A2	3536	P7G	C8-N7	6.36	1.51	1.45
9	A2	398	A2M	O4'-C1'	-6.36	1.32	1.41
9	A2	4135	B8T	C2-N3	6.36	1.49	1.36
9	A2	1673	A2M	O4'-C1'	-6.36	1.32	1.41
9	A2	4023	MHG	C2-N1	6.34	1.46	1.36
9	A2	3374	A2M	O4'-C1'	-6.33	1.32	1.41
9	A2	4188	OMC	C2-N3	6.32	1.49	1.36
9	A2	237	B9B	O6-C6	6.30	1.40	1.35
9	A2	3525	OMC	C2-N3	6.28	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3846	I4U	C6-C5	6.25	1.49	1.35
9	A2	3543	OMC	C6-C5	6.21	1.49	1.35
9	A2	2052	E7G	C8-N7	6.20	1.51	1.45
9	A2	1599	E7G	C8-N7	6.19	1.51	1.45
9	A2	1472	I4U	C2-N3	6.19	1.48	1.36
9	A2	3438	5MC	C2-N3	6.18	1.48	1.36
9	A2	2541	B9H	C2-N1	6.18	1.47	1.38
9	A2	1472	I4U	C6-C5	6.16	1.49	1.35
9	A2	3987	5MC	C2-N3	6.12	1.48	1.36
9	A2	3846	I4U	C2-N3	6.10	1.48	1.36
9	A2	4099	5MC	C2-N3	6.09	1.48	1.36
9	A2	4135	B8T	C6-C5	6.09	1.49	1.35
9	A2	2177	OMC	C6-C5	6.04	1.49	1.35
46	m2	1832	UR3	C6-C5	6.03	1.49	1.35
46	m2	519	OMC	C6-C5	6.01	1.49	1.35
9	A2	3357	OMC	C6-C5	5.99	1.49	1.35
9	A2	3543	OMC	C2-N3	5.99	1.48	1.36
9	A2	1387	B9B	O6-C6	5.98	1.40	1.35
9	A2	2616	OMC	C6-C5	5.98	1.49	1.35
9	A2	4188	OMC	C6-C5	5.98	1.49	1.35
9	A2	1599	E7G	C2-N3	5.96	1.47	1.33
9	A2	1668	UR3	C6-C5	5.96	1.48	1.35
9	A2	2052	E7G	C2-N3	5.94	1.47	1.33
9	A2	3525	OMC	C6-C5	5.94	1.48	1.35
46	m2	1250	B8N	C6-C5	5.94	1.43	1.34
9	A2	2559	OMC	C6-C5	5.93	1.48	1.35
9	A2	1269	B8Q	C2-N1	5.92	1.47	1.38
9	A2	4007	E6G	O6-C6	5.90	1.40	1.35
9	A2	3565	OMC	C6-C5	5.89	1.48	1.35
9	A2	4249	UR3	C6-C5	5.89	1.48	1.35
9	A2	1418	G7M	C2-N3	5.88	1.47	1.33
9	A2	237	B9B	C2-N2	5.85	1.45	1.33
9	A2	2120	OMC	C6-C5	5.83	1.48	1.35
9	A2	2277	G7M	C2-N3	5.82	1.47	1.33
9	A2	4202	G7M	C2-N3	5.81	1.47	1.33
9	A2	1387	B9B	C2-N2	5.80	1.45	1.33
9	A2	4007	E6G	C2-N2	5.78	1.45	1.33
46	m2	1250	B8N	C2-N1	5.73	1.56	1.39
11	C2	14	OMU	C6-C5	5.69	1.48	1.35
9	A2	1599	E7G	C4-N9	5.67	1.44	1.37
9	A2	3958	OMU	C6-C5	5.66	1.48	1.35
9	A2	4272	OMU	C6-C5	5.64	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	m2	116	OMU	C6-C5	5.63	1.48	1.35
9	A2	3536	P7G	C2-N1	5.61	1.46	1.33
9	A2	2528	OMG	C2-N3	5.55	1.46	1.33
46	m2	646	OMG	C2-N3	5.51	1.46	1.33
9	A2	1711	P7G	C2-N1	5.51	1.46	1.33
9	A2	2179	OMG	C2-N3	5.50	1.46	1.33
9	A2	4146	OMG	C2-N3	5.50	1.46	1.33
9	A2	4515	OMG	C2-N3	5.49	1.46	1.33
9	A2	1438	OMG	C2-N3	5.49	1.46	1.33
9	A2	3448	OMG	C2-N3	5.48	1.46	1.33
9	A2	4022	OMG	C2-N3	5.48	1.46	1.33
9	A2	4275	OMG	C2-N3	5.44	1.46	1.33
9	A2	3848	OMG	C2-N3	5.44	1.46	1.33
9	A2	4289	OMG	C2-N3	5.44	1.46	1.33
9	A2	1685	OMG	C2-N3	5.44	1.46	1.33
9	A2	3846	I4U	O4'-C1'	-5.43	1.29	1.42
46	m2	685	OMG	C2-N3	5.43	1.46	1.33
9	A2	1852	OMG	C2-N3	5.42	1.46	1.33
9	A2	2052	E7G	C4-N9	5.40	1.44	1.37
9	A2	1335	OMG	C2-N3	5.40	1.46	1.33
9	A2	2119	OMG	C2-N3	5.36	1.46	1.33
9	A2	3565	OMC	C4-N3	5.36	1.45	1.34
9	A2	373	OMG	C2-N3	5.35	1.46	1.33
9	A2	3357	OMC	C4-N3	5.31	1.45	1.34
9	A2	4249	UR3	C2-N3	5.28	1.49	1.39
46	m2	1832	UR3	C2-N3	5.28	1.49	1.39
46	m2	519	OMC	C4-N3	5.24	1.45	1.34
9	A2	2616	OMC	C4-N3	5.24	1.45	1.34
9	A2	2559	OMC	C4-N3	5.21	1.45	1.34
9	A2	1668	UR3	C2-N3	5.21	1.49	1.39
9	A2	1490	PSU	C6-N1	5.19	1.44	1.36
9	A2	3525	OMC	C4-N3	5.19	1.45	1.34
9	A2	4288	PSU	C6-N1	5.17	1.44	1.36
9	A2	3543	OMC	C4-N3	5.16	1.44	1.34
46	m2	825	PSU	C6-N1	5.16	1.44	1.36
9	A2	2263	PSU	C6-N1	5.15	1.44	1.36
9	A2	3385	PSU	C6-N1	5.15	1.44	1.36
9	A2	2177	OMC	C4-N3	5.14	1.44	1.34
9	A2	3543	OMC	C4-N4	5.14	1.46	1.33
9	A2	1472	I4U	O4'-C1'	-5.13	1.29	1.42
9	A2	2120	OMC	C4-N3	5.13	1.44	1.34
9	A2	4188	OMC	C4-N3	5.13	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	4055	PSU	C6-N1	5.11	1.44	1.36
9	A2	4102	PSU	C6-N1	5.11	1.44	1.36
9	A2	3420	PSU	C6-N1	5.11	1.44	1.36
9	A2	4152	PSU	C6-N1	5.10	1.44	1.36
9	A2	1711	P7G	C2-N2	5.09	1.46	1.34
9	A2	3536	P7G	C2-N2	5.09	1.46	1.34
46	m2	1245	PSU	C6-N1	5.09	1.44	1.36
46	m2	614	PSU	C6-N1	5.09	1.44	1.36
9	A2	1496	PSU	C6-N1	5.08	1.44	1.36
9	A2	4094	PSU	C6-N1	5.08	1.44	1.36
46	m2	1083	PSU	C6-N1	5.08	1.44	1.36
9	A2	4280	PSU	C6-N1	5.07	1.44	1.36
9	A2	3371	PSU	C6-N1	5.06	1.44	1.36
9	A2	4183	PSU	C6-N1	5.05	1.44	1.36
9	A2	3945	PSU	C6-N1	5.05	1.44	1.36
9	A2	878	2MG	C4-N3	5.05	1.49	1.37
9	A2	1395	PSU	C6-N1	5.04	1.44	1.36
9	A2	2528	OMG	C4-N3	5.04	1.49	1.37
9	A2	2120	OMC	C2-N1	5.03	1.50	1.40
79	m	714	DDE	CBI-NAD	5.02	1.45	1.32
9	A2	3448	OMG	C4-N3	4.99	1.49	1.37
46	m2	646	OMG	C4-N3	4.99	1.49	1.37
9	A2	2179	OMG	C4-N3	4.98	1.49	1.37
9	A2	1685	OMG	C4-N3	4.97	1.49	1.37
9	A2	4146	OMG	C4-N3	4.97	1.49	1.37
9	A2	1438	OMG	C4-N3	4.97	1.49	1.37
9	A2	4517	2MG	C4-N3	4.95	1.49	1.37
46	m2	685	OMG	C4-N3	4.95	1.49	1.37
9	A2	4515	OMG	C4-N3	4.95	1.49	1.37
9	A2	3848	OMG	C4-N3	4.95	1.49	1.37
9	A2	4022	OMG	C4-N3	4.94	1.49	1.37
9	A2	4275	OMG	C4-N3	4.94	1.49	1.37
9	A2	4289	OMG	C4-N3	4.93	1.49	1.37
9	A2	1330	2MG	C2-N1	4.92	1.44	1.36
9	A2	1852	OMG	C4-N3	4.92	1.49	1.37
9	A2	1330	2MG	C4-N3	4.92	1.49	1.37
9	A2	1335	OMG	C4-N3	4.91	1.49	1.37
9	A2	3565	OMC	C4-N4	4.89	1.45	1.33
9	A2	373	OMG	C4-N3	4.88	1.49	1.37
9	A2	3525	OMC	C4-N4	4.88	1.45	1.33
46	m2	646	OMG	C2-N2	4.87	1.45	1.34
9	A2	2177	OMC	C4-N4	4.87	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	4188	OMC	C4-N4	4.86	1.45	1.33
9	A2	2119	OMG	C4-N3	4.86	1.49	1.37
9	A2	878	2MG	C2-N1	4.86	1.44	1.36
9	A2	2616	OMC	C2-N1	4.86	1.50	1.40
9	A2	2616	OMC	C4-N4	4.85	1.45	1.33
46	m2	519	OMC	C4-N4	4.85	1.45	1.33
9	A2	4515	OMG	C2-N2	4.85	1.45	1.34
46	m2	824	PSU	C6-N1	4.84	1.44	1.36
9	A2	2120	OMC	C4-N4	4.84	1.45	1.33
46	m2	519	OMC	C2-N1	4.83	1.50	1.40
9	A2	2528	OMG	C2-N2	4.83	1.45	1.34
9	A2	4517	2MG	C2-N1	4.82	1.44	1.36
9	A2	3357	OMC	C4-N4	4.82	1.45	1.33
46	m2	685	OMG	C2-N2	4.82	1.45	1.34
9	A2	2179	OMG	C2-N2	4.81	1.45	1.34
9	A2	2559	OMC	C4-N4	4.81	1.45	1.33
9	A2	1685	OMG	C2-N2	4.81	1.45	1.34
9	A2	1335	OMG	C2-N2	4.81	1.45	1.34
9	A2	373	OMG	C2-N2	4.81	1.45	1.34
9	A2	1438	OMG	C2-N2	4.80	1.45	1.34
9	A2	4146	OMG	C2-N2	4.80	1.45	1.34
9	A2	1472	I4U	C5-C4	4.80	1.49	1.43
9	A2	3848	OMG	C2-N2	4.79	1.45	1.34
9	A2	4022	OMG	C2-N2	4.79	1.45	1.34
9	A2	3448	OMG	C2-N2	4.79	1.45	1.34
9	A2	2052	E7G	C2-N2	4.78	1.45	1.34
9	A2	3846	I4U	C5-C4	4.78	1.49	1.43
9	A2	4275	OMG	C2-N2	4.77	1.45	1.34
9	A2	1852	OMG	C2-N2	4.76	1.45	1.34
46	m2	1844	4AC	C2-N1	4.76	1.50	1.40
9	A2	2119	OMG	C2-N2	4.75	1.45	1.34
9	A2	4289	OMG	C2-N2	4.74	1.45	1.34
9	A2	1599	E7G	C2-N2	4.73	1.45	1.34
9	A2	4135	B8T	C4-N4	4.69	1.45	1.35
9	A2	2277	G7M	C2-N2	4.69	1.45	1.34
9	A2	2277	G7M	C6-N1	4.67	1.44	1.37
9	A2	1418	G7M	C6-N1	4.66	1.44	1.37
9	A2	1418	G7M	C2-N2	4.65	1.45	1.34
9	A2	4202	G7M	C6-N1	4.65	1.44	1.37
9	A2	4202	G7M	C2-N2	4.65	1.45	1.34
9	A2	3438	5MC	C6-N1	4.63	1.45	1.38
46	m2	1844	4AC	C5-C4	4.62	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	1472	I4U	C2'-C1'	4.59	1.68	1.53
46	m2	824	PSU	C4-N3	4.56	1.47	1.38
9	A2	4099	5MC	C6-N1	4.56	1.45	1.38
9	A2	3565	OMC	C2-N1	4.56	1.49	1.40
9	A2	4188	OMC	C2-N1	4.55	1.49	1.40
9	A2	3525	OMC	C2-N1	4.53	1.49	1.40
9	A2	2559	OMC	C2-N1	4.53	1.49	1.40
9	A2	3536	P7G	C2-N3	4.47	1.48	1.37
9	A2	3357	OMC	C2-N1	4.46	1.49	1.40
9	A2	3846	I4U	C2'-C1'	4.44	1.67	1.53
9	A2	3846	I4U	O4'-C4'	4.42	1.54	1.45
9	A2	3837	B8W	C2-N2	4.41	1.42	1.33
9	A2	3987	5MC	C6-N1	4.41	1.45	1.38
9	A2	1472	I4U	O4'-C4'	4.39	1.54	1.45
9	A2	3543	OMC	C2-N1	4.38	1.49	1.40
9	A2	3438	5MC	C4-N4	4.38	1.45	1.34
9	A2	1711	P7G	C2-N3	4.37	1.48	1.37
9	A2	3987	5MC	C4-N4	4.34	1.45	1.34
9	A2	4099	5MC	C4-N4	4.34	1.45	1.34
9	A2	3837	B8W	O3'-C3'	-4.33	1.32	1.43
9	A2	1472	I4U	C5'-C4'	-4.29	1.38	1.51
9	A2	3846	I4U	C5'-C4'	-4.29	1.38	1.51
9	A2	4135	B8T	C2-N1	4.27	1.49	1.40
9	A2	2177	OMC	C2-N1	4.27	1.49	1.40
46	m2	1844	4AC	C7-N4	4.26	1.45	1.37
9	A2	4099	5MC	C2-N1	4.20	1.49	1.40
46	m2	614	PSU	C4-N3	4.18	1.46	1.38
9	A2	3987	5MC	C2-N1	4.17	1.49	1.40
9	A2	4067	1MA	C2-N1	4.15	1.43	1.35
9	A2	1472	I4U	C2-N1	4.13	1.49	1.40
9	A2	3385	PSU	C4-N3	4.12	1.46	1.38
9	A2	4094	PSU	C4-N3	4.11	1.46	1.38
46	m2	116	OMU	C4-N3	4.10	1.45	1.38
9	A2	3420	PSU	C4-N3	4.10	1.46	1.38
11	C2	14	OMU	C4-N3	4.09	1.45	1.38
9	A2	3945	PSU	C4-N3	4.09	1.46	1.38
9	A2	4152	PSU	C4-N3	4.09	1.46	1.38
9	A2	4288	PSU	C4-N3	4.08	1.46	1.38
9	A2	3846	I4U	C2-N1	4.08	1.48	1.40
9	A2	1490	PSU	C4-N3	4.08	1.46	1.38
9	A2	2263	PSU	C4-N3	4.07	1.46	1.38
9	A2	3371	PSU	C4-N3	4.06	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	4280	PSU	C4-N3	4.05	1.46	1.38
46	m2	825	PSU	C4-N3	4.05	1.46	1.38
9	A2	4102	PSU	C4-N3	4.05	1.46	1.38
9	A2	4055	PSU	C4-N3	4.04	1.46	1.38
46	m2	1083	PSU	C4-N3	4.04	1.46	1.38
9	A2	1395	PSU	C4-N3	4.04	1.46	1.38
9	A2	4183	PSU	C4-N3	4.04	1.46	1.38
9	A2	1668	UR3	O4-C4	-4.04	1.14	1.23
9	A2	3958	OMU	C4-N3	4.02	1.45	1.38
9	A2	1496	PSU	C4-N3	4.01	1.46	1.38
9	A2	3438	5MC	C2-N1	4.00	1.48	1.40
9	A2	4249	UR3	O4-C4	-3.98	1.15	1.23
9	A2	4272	OMU	C4-N3	3.98	1.45	1.38
46	m2	1245	PSU	C4-N3	3.96	1.46	1.38
46	m2	1832	UR3	O4-C4	-3.94	1.15	1.23
9	A2	4135	B8T	C5-C4	3.87	1.49	1.40
9	A2	398	A2M	C6-N6	3.83	1.48	1.34
46	m2	27	A2M	C6-N6	3.82	1.48	1.34
46	m2	166	A2M	C6-N6	3.82	1.48	1.34
9	A2	3374	A2M	C6-N6	3.81	1.48	1.34
9	A2	3481	A2M	C6-N6	3.81	1.48	1.34
9	A2	373	OMG	C6-N1	3.80	1.43	1.37
46	m2	670	A2M	C6-N6	3.80	1.47	1.34
9	A2	3379	A2M	C6-N6	3.80	1.47	1.34
9	A2	3523	A2M	C6-N6	3.80	1.47	1.34
9	A2	2118	A2M	C6-N6	3.79	1.47	1.34
9	A2	3848	OMG	C6-N1	3.79	1.43	1.37
9	A2	2119	OMG	C6-N1	3.79	1.43	1.37
9	A2	4223	A2M	C6-N6	3.79	1.47	1.34
9	A2	1673	A2M	C6-N6	3.79	1.47	1.34
9	A2	1337	A2M	C6-N6	3.79	1.47	1.34
46	m2	1033	A2M	C6-N6	3.78	1.47	1.34
9	A2	2156	A2M	C6-N6	3.78	1.47	1.34
9	A2	1347	A2M	C6-N6	3.77	1.47	1.34
9	A2	1140	A2M	C6-N6	3.77	1.47	1.34
9	A2	1335	OMG	C6-N1	3.76	1.43	1.37
46	m2	685	OMG	C6-N1	3.76	1.43	1.37
9	A2	2179	OMG	C6-N1	3.75	1.43	1.37
9	A2	4515	OMG	C6-N1	3.75	1.43	1.37
9	A2	4275	OMG	C6-N1	3.74	1.43	1.37
9	A2	1852	OMG	C6-N1	3.73	1.43	1.37
9	A2	3441	A2M	C6-N6	3.73	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	1685	OMG	C6-N1	3.72	1.43	1.37
9	A2	2277	G7M	C2-N1	3.72	1.46	1.37
9	A2	2528	OMG	C6-N1	3.72	1.43	1.37
9	A2	4022	OMG	C6-N1	3.71	1.43	1.37
9	A2	4202	G7M	C2-N1	3.71	1.46	1.37
9	A2	237	B9B	O2'-C2'	3.71	1.51	1.43
9	A2	1418	G7M	C2-N1	3.70	1.46	1.37
9	A2	4007	E6G	O2'-C2'	3.69	1.51	1.43
9	A2	1387	B9B	O2'-C2'	3.68	1.51	1.43
46	m2	646	OMG	C6-N1	3.67	1.43	1.37
9	A2	4289	OMG	C6-N1	3.66	1.43	1.37
9	A2	4146	OMG	C6-N1	3.66	1.43	1.37
9	A2	3448	OMG	C6-N1	3.66	1.43	1.37
9	A2	1438	OMG	C6-N1	3.65	1.43	1.37
9	A2	1330	2MG	C6-N1	3.65	1.43	1.37
9	A2	1599	E7G	C2-N1	3.64	1.46	1.37
9	A2	2052	E7G	C2-N1	3.62	1.46	1.37
9	A2	3536	P7G	C5-C4	3.62	1.44	1.37
9	A2	2177	OMC	C6-N1	3.61	1.46	1.38
9	A2	4023	MHG	C5-C6	3.59	1.52	1.43
9	A2	1711	P7G	C5-C4	3.58	1.44	1.37
9	A2	4517	2MG	C6-N1	3.57	1.43	1.37
9	A2	3536	P7G	C6-N1	3.55	1.44	1.38
9	A2	1711	P7G	C6-N1	3.53	1.44	1.38
9	A2	1599	E7G	C5-C6	3.50	1.52	1.43
9	A2	878	2MG	C6-N1	3.50	1.43	1.37
9	A2	4289	OMG	C5-C6	3.49	1.54	1.47
9	A2	2120	OMC	C6-N1	3.48	1.46	1.38
9	A2	3543	OMC	C6-N1	3.47	1.46	1.38
9	A2	2052	E7G	C5-C6	3.45	1.52	1.43
9	A2	1337	A2M	C5'-C4'	-3.44	1.40	1.51
9	A2	3374	A2M	C5'-C4'	-3.43	1.40	1.51
9	A2	3523	A2M	C5'-C4'	-3.42	1.40	1.51
46	m2	670	A2M	C5'-C4'	-3.40	1.41	1.51
9	A2	1140	A2M	C5'-C4'	-3.39	1.41	1.51
9	A2	3481	A2M	C5'-C4'	-3.38	1.41	1.51
46	m2	1033	A2M	C5'-C4'	-3.38	1.41	1.51
9	A2	2156	A2M	C5'-C4'	-3.37	1.41	1.51
9	A2	4223	A2M	C5'-C4'	-3.36	1.41	1.51
9	A2	3525	OMC	C6-N1	3.34	1.46	1.38
9	A2	398	A2M	C5'-C4'	-3.34	1.41	1.51
9	A2	3441	A2M	C5'-C4'	-3.34	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3379	A2M	C5'-C4'	-3.31	1.41	1.51
9	A2	4188	OMC	C6-N1	3.31	1.46	1.38
9	A2	1347	A2M	C5'-C4'	-3.30	1.41	1.51
46	m2	519	OMC	C6-N1	3.30	1.46	1.38
46	m2	166	A2M	C5'-C4'	-3.30	1.41	1.51
9	A2	2616	OMC	C6-N1	3.30	1.46	1.38
46	m2	27	A2M	C5'-C4'	-3.29	1.41	1.51
9	A2	1673	A2M	C5'-C4'	-3.29	1.41	1.51
9	A2	2559	OMC	C6-N1	3.28	1.45	1.38
9	A2	3441	A2M	C3'-C4'	3.28	1.61	1.53
9	A2	1711	P7G	O6-C6	-3.28	1.18	1.23
9	A2	3565	OMC	C6-N1	3.27	1.45	1.38
9	A2	3357	OMC	C6-N1	3.26	1.45	1.38
9	A2	3536	P7G	O6-C6	-3.25	1.18	1.23
9	A2	2118	A2M	C5'-C4'	-3.24	1.41	1.51
9	A2	3846	I4U	C6-N1	3.15	1.45	1.38
9	A2	1347	A2M	C3'-C4'	3.14	1.61	1.53
9	A2	3837	B8W	C5-C4	-3.13	1.32	1.40
9	A2	4135	B8T	C6-N1	3.12	1.45	1.38
46	m2	1844	4AC	C6-N1	3.12	1.45	1.38
46	m2	1832	UR3	C5-C4	3.11	1.51	1.43
9	A2	1472	I4U	C6-N1	3.11	1.45	1.38
9	A2	3523	A2M	C3'-C4'	3.10	1.60	1.53
9	A2	1335	OMG	C5-C6	3.10	1.53	1.47
9	A2	2179	OMG	C5-C6	3.10	1.53	1.47
46	m2	646	OMG	C5-C6	3.10	1.53	1.47
9	A2	1599	E7G	C6-N1	3.10	1.44	1.38
46	m2	166	A2M	C3'-C4'	3.10	1.60	1.53
9	A2	1330	2MG	C5-C6	3.09	1.53	1.47
9	A2	4275	OMG	C5-C6	3.07	1.53	1.47
46	m2	685	OMG	C5-C6	3.06	1.53	1.47
9	A2	3848	OMG	C5-C6	3.05	1.53	1.47
9	A2	2119	OMG	C5-C6	3.05	1.53	1.47
9	A2	1668	UR3	C5-C4	3.04	1.51	1.43
9	A2	3846	I4U	O4-C41	-3.04	1.40	1.47
9	A2	4249	UR3	C5-C4	3.02	1.51	1.43
79	m	714	DDE	CD2-NE2	-3.02	1.31	1.36
9	A2	4022	OMG	C5-C6	3.02	1.53	1.47
9	A2	2156	A2M	C3'-C4'	3.01	1.60	1.53
46	m2	670	A2M	O3'-C3'	3.01	1.50	1.43
9	A2	1852	OMG	C5-C6	3.01	1.53	1.47
9	A2	2118	A2M	C3'-C4'	3.01	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	373	OMG	C5-C6	3.01	1.53	1.47
9	A2	1140	A2M	C3'-C4'	3.00	1.60	1.53
9	A2	4517	2MG	C5-C6	3.00	1.53	1.47
9	A2	878	2MG	C5-C6	2.99	1.53	1.47
9	A2	1438	OMG	C5-C6	2.98	1.53	1.47
9	A2	4146	OMG	C5-C6	2.98	1.53	1.47
46	m2	27	A2M	C3'-C4'	2.98	1.60	1.53
11	C2	14	OMU	O4-C4	-2.97	1.18	1.24
46	m2	1033	A2M	C3'-C4'	2.97	1.60	1.53
9	A2	1472	I4U	O4-C41	-2.97	1.40	1.47
9	A2	2528	OMG	C5-C6	2.96	1.53	1.47
9	A2	2052	E7G	C6-N1	2.96	1.44	1.38
9	A2	3448	OMG	C5-C6	2.96	1.53	1.47
9	A2	398	A2M	C3'-C4'	2.96	1.60	1.53
9	A2	1472	I4U	O3'-C3'	2.96	1.49	1.43
46	m2	166	A2M	O3'-C3'	2.96	1.49	1.43
46	m2	670	A2M	C3'-C4'	2.95	1.60	1.53
9	A2	3379	A2M	O2'-C2'	2.95	1.50	1.42
9	A2	3958	OMU	O4-C4	-2.95	1.18	1.24
9	A2	3837	B8W	C3'-C4'	2.95	1.60	1.53
9	A2	4272	OMU	O4-C4	-2.94	1.18	1.24
9	A2	3379	A2M	C3'-C4'	2.94	1.60	1.53
9	A2	3481	A2M	C3'-C4'	2.93	1.60	1.53
46	m2	116	OMU	O4-C4	-2.93	1.18	1.24
9	A2	2156	A2M	O3'-C3'	2.92	1.49	1.43
9	A2	4223	A2M	C3'-C4'	2.92	1.60	1.53
9	A2	1387	B9B	O3'-C3'	-2.92	1.36	1.43
9	A2	1685	OMG	C5-C6	2.92	1.53	1.47
9	A2	1140	A2M	O2'-C2'	2.92	1.50	1.42
46	m2	27	A2M	O2'-C2'	2.92	1.50	1.42
9	A2	4007	E6G	O3'-C3'	-2.91	1.36	1.43
46	m2	1033	A2M	O2'-C2'	2.91	1.50	1.42
9	A2	3441	A2M	O3'-C3'	2.91	1.49	1.43
9	A2	398	A2M	O2'-C2'	2.90	1.50	1.42
46	m2	166	A2M	O2'-C2'	2.90	1.50	1.42
9	A2	3846	I4U	O3'-C3'	2.89	1.49	1.43
9	A2	4515	OMG	C5-C6	2.88	1.53	1.47
9	A2	1337	A2M	O2'-C2'	2.88	1.50	1.42
9	A2	2118	A2M	O3'-C3'	2.88	1.49	1.43
9	A2	4067	1MA	C5-C4	-2.87	1.35	1.43
46	m2	1033	A2M	O3'-C3'	2.87	1.49	1.43
9	A2	3379	A2M	O3'-C3'	2.87	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3523	A2M	O3'-C3'	2.87	1.49	1.43
9	A2	4223	A2M	O2'-C2'	2.87	1.50	1.42
9	A2	398	A2M	O3'-C3'	2.87	1.49	1.43
9	A2	3374	A2M	C3'-C4'	2.87	1.60	1.53
46	m2	27	A2M	O3'-C3'	2.87	1.49	1.43
9	A2	1140	A2M	O3'-C3'	2.86	1.49	1.43
9	A2	1347	A2M	O2'-C2'	2.86	1.50	1.42
9	A2	3481	A2M	O2'-C2'	2.86	1.50	1.42
9	A2	3374	A2M	O2'-C2'	2.86	1.50	1.42
9	A2	3523	A2M	O2'-C2'	2.86	1.49	1.42
9	A2	4023	MHG	C6-N1	2.86	1.44	1.38
46	m2	670	A2M	O2'-C2'	2.86	1.49	1.42
9	A2	4223	A2M	O3'-C3'	2.85	1.49	1.43
9	A2	2156	A2M	O2'-C2'	2.85	1.49	1.42
11	C2	14	OMU	C6-N1	2.85	1.44	1.38
9	A2	1673	A2M	O2'-C2'	2.85	1.49	1.42
9	A2	3481	A2M	O3'-C3'	2.84	1.49	1.43
9	A2	2118	A2M	O2'-C2'	2.84	1.49	1.42
9	A2	3441	A2M	O2'-C2'	2.83	1.49	1.42
9	A2	1673	A2M	C3'-C4'	2.83	1.60	1.53
9	A2	1337	A2M	O3'-C3'	2.83	1.49	1.43
9	A2	1347	A2M	O3'-C3'	2.82	1.49	1.43
9	A2	1337	A2M	C3'-C4'	2.82	1.60	1.53
9	A2	3374	A2M	O3'-C3'	2.82	1.49	1.43
46	m2	116	OMU	C6-N1	2.82	1.44	1.38
46	m2	1832	UR3	C6-N1	2.81	1.44	1.38
9	A2	3958	OMU	C6-N1	2.81	1.44	1.38
9	A2	237	B9B	O3'-C3'	-2.80	1.36	1.43
46	m2	166	A2M	O4'-C4'	2.80	1.51	1.45
9	A2	2528	OMG	C2-N1	2.80	1.44	1.37
9	A2	1668	UR3	C6-N1	2.79	1.44	1.38
9	A2	2119	OMG	C2-N1	2.79	1.44	1.37
9	A2	3374	A2M	O4'-C4'	2.79	1.51	1.45
9	A2	2156	A2M	O4'-C4'	2.79	1.51	1.45
46	m2	646	OMG	C2-N1	2.79	1.44	1.37
9	A2	373	OMG	C2-N1	2.78	1.44	1.37
9	A2	2179	OMG	C2-N1	2.78	1.44	1.37
9	A2	1673	A2M	O4'-C4'	2.78	1.51	1.45
9	A2	4515	OMG	C2-N1	2.77	1.44	1.37
46	m2	685	OMG	C2-N1	2.77	1.44	1.37
9	A2	2177	OMC	O2-C2	-2.77	1.18	1.23
9	A2	1673	A2M	O3'-C3'	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3848	OMG	C2-N1	2.76	1.44	1.37
9	A2	4275	OMG	C2-N1	2.75	1.44	1.37
9	A2	1685	OMG	C2-N1	2.75	1.44	1.37
9	A2	3837	B8W	O2'-C2'	2.75	1.49	1.43
9	A2	1335	OMG	C2-N1	2.74	1.44	1.37
46	m2	1844	4AC	O7-C7	-2.74	1.17	1.23
9	A2	1438	OMG	C2-N1	2.74	1.44	1.37
9	A2	4272	OMU	C6-N1	2.73	1.44	1.38
9	A2	398	A2M	O4'-C4'	2.73	1.51	1.45
9	A2	3523	A2M	O4'-C4'	2.73	1.51	1.45
9	A2	4146	OMG	C2-N1	2.73	1.44	1.37
9	A2	3448	OMG	C2-N1	2.72	1.44	1.37
9	A2	2616	OMC	O2-C2	-2.72	1.18	1.23
9	A2	2118	A2M	O4'-C4'	2.72	1.51	1.45
9	A2	1387	B9B	C5-C4	-2.72	1.33	1.40
9	A2	3846	I4U	O2-C2	-2.71	1.18	1.23
46	m2	1033	A2M	O4'-C4'	2.71	1.51	1.45
9	A2	1852	OMG	C2-N1	2.71	1.44	1.37
9	A2	1472	I4U	O2-C2	-2.70	1.18	1.23
9	A2	4223	A2M	O4'-C4'	2.70	1.51	1.45
9	A2	4022	OMG	C2-N1	2.70	1.44	1.37
9	A2	2559	OMC	O2-C2	-2.69	1.18	1.23
9	A2	4135	B8T	O2-C2	-2.69	1.18	1.23
9	A2	4202	G7M	C5-C6	2.69	1.52	1.45
9	A2	4249	UR3	C6-N1	2.69	1.44	1.38
9	A2	3525	OMC	O2-C2	-2.69	1.18	1.23
9	A2	3872	6MZ	C5-C4	-2.68	1.33	1.40
9	A2	373	OMG	C5-C4	-2.68	1.36	1.43
9	A2	1418	G7M	C5-C6	2.68	1.52	1.45
9	A2	1269	B8Q	C6-N1	2.68	1.44	1.38
9	A2	4007	E6G	C5-C4	-2.67	1.33	1.40
9	A2	4289	OMG	C2-N1	2.67	1.44	1.37
9	A2	3438	5MC	O2-C2	-2.66	1.18	1.23
9	A2	3379	A2M	O4'-C4'	2.66	1.50	1.45
9	A2	4188	OMC	O2-C2	-2.65	1.18	1.23
9	A2	2277	G7M	C5-C6	2.65	1.52	1.45
46	m2	27	A2M	O4'-C4'	2.65	1.50	1.45
9	A2	3565	OMC	O2-C2	-2.65	1.18	1.23
9	A2	3987	5MC	O2-C2	-2.65	1.18	1.23
9	A2	1335	OMG	C5-C4	-2.64	1.36	1.43
9	A2	3481	A2M	O4'-C4'	2.64	1.50	1.45
9	A2	1347	A2M	O4'-C4'	2.64	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3357	OMC	O2-C2	-2.64	1.18	1.23
9	A2	3543	OMC	O2-C2	-2.64	1.18	1.23
9	A2	1685	OMG	C5-C4	-2.64	1.36	1.43
9	A2	1418	G7M	C5-C4	2.62	1.44	1.39
46	m2	519	OMC	O2-C2	-2.62	1.18	1.23
9	A2	1852	OMG	C5-C4	-2.61	1.36	1.43
9	A2	2119	OMG	C5-C4	-2.61	1.36	1.43
9	A2	1472	I4U	O4-C4	2.60	1.40	1.35
9	A2	4275	OMG	C5-C4	-2.60	1.36	1.43
9	A2	3565	OMC	C5-C4	2.60	1.48	1.42
9	A2	3543	OMC	C5-C4	2.59	1.48	1.42
9	A2	1140	A2M	O4'-C4'	2.59	1.50	1.45
9	A2	4022	OMG	C5-C4	-2.59	1.36	1.43
9	A2	2277	G7M	C5-C4	2.59	1.44	1.39
9	A2	3848	OMG	C5-C4	-2.59	1.36	1.43
9	A2	3441	A2M	O4'-C4'	2.58	1.50	1.45
9	A2	237	B9B	C5-C4	-2.58	1.34	1.40
46	m2	685	OMG	C5-C4	-2.58	1.36	1.43
9	A2	1330	2MG	C5-C4	-2.58	1.36	1.43
9	A2	2052	E7G	O6-C6	-2.58	1.18	1.23
9	A2	4146	OMG	C5-C4	-2.58	1.36	1.43
9	A2	4099	5MC	O2-C2	-2.57	1.18	1.23
9	A2	1599	E7G	O6-C6	-2.56	1.18	1.23
9	A2	3448	OMG	C5-C4	-2.55	1.36	1.43
9	A2	4094	PSU	O4'-C1'	-2.55	1.40	1.43
9	A2	1438	OMG	C5-C4	-2.55	1.36	1.43
9	A2	4202	G7M	C5-C4	2.55	1.44	1.39
9	A2	2179	OMG	C5-C4	-2.54	1.36	1.43
9	A2	4517	2MG	C5-C4	-2.54	1.36	1.43
46	m2	646	OMG	C5-C4	-2.53	1.36	1.43
9	A2	878	2MG	C5-C4	-2.53	1.36	1.43
46	m2	670	A2M	O4'-C4'	2.51	1.50	1.45
9	A2	2528	OMG	C5-C4	-2.51	1.36	1.43
79	m	714	DDE	OAG-CBI	-2.50	1.19	1.23
46	m2	519	OMC	C5-C4	2.50	1.48	1.42
9	A2	3357	OMC	C5-C4	2.50	1.48	1.42
9	A2	3846	I4U	O4-C4	2.50	1.40	1.35
9	A2	2541	B9H	C6-N1	2.48	1.44	1.38
9	A2	1337	A2M	O4'-C4'	2.47	1.50	1.45
9	A2	4188	OMC	C5-C4	2.47	1.48	1.42
11	C2	14	OMU	C5-C4	2.47	1.49	1.43
9	A2	3420	PSU	C1'-C5	2.47	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3525	OMC	C5-C4	2.46	1.48	1.42
46	m2	1832	UR3	O2-C2	-2.46	1.18	1.22
9	A2	2559	OMC	C5-C4	2.46	1.48	1.42
9	A2	2177	OMC	C5-C4	2.45	1.48	1.42
9	A2	2616	OMC	C5-C4	2.45	1.48	1.42
9	A2	4289	OMG	C5-C4	-2.45	1.36	1.43
9	A2	3374	A2M	C2-N3	2.45	1.36	1.32
46	m2	166	A2M	C2-N3	2.44	1.36	1.32
9	A2	1347	A2M	C2-N3	2.43	1.36	1.32
9	A2	1337	A2M	C2-N3	2.42	1.36	1.32
46	m2	824	PSU	C1'-C5	2.42	1.55	1.50
9	A2	4515	OMG	C5-C4	-2.42	1.36	1.43
9	A2	4223	A2M	C2-N3	2.41	1.36	1.32
9	A2	1668	UR3	O2-C2	-2.41	1.18	1.22
9	A2	3846	I4U	C3'-C4'	2.40	1.59	1.53
9	A2	3371	PSU	C1'-C5	2.39	1.55	1.50
9	A2	4094	PSU	C1'-C5	2.39	1.55	1.50
9	A2	1673	A2M	C2-N3	2.39	1.35	1.32
9	A2	4249	UR3	O2-C2	-2.39	1.18	1.22
46	m2	27	A2M	C2-N3	2.39	1.35	1.32
46	m2	670	A2M	C2-N3	2.38	1.35	1.32
9	A2	398	A2M	C2-N3	2.38	1.35	1.32
9	A2	3379	A2M	C2-N3	2.38	1.35	1.32
9	A2	2118	A2M	C2-N3	2.37	1.35	1.32
9	A2	2263	PSU	C1'-C5	2.37	1.55	1.50
9	A2	3481	A2M	C2-N3	2.37	1.35	1.32
9	A2	4202	G7M	O6-C6	-2.36	1.18	1.23
9	A2	1140	A2M	C2-N3	2.35	1.35	1.32
46	m2	1033	A2M	C2-N3	2.35	1.35	1.32
9	A2	2277	G7M	O6-C6	-2.35	1.18	1.23
9	A2	3441	A2M	C2-N3	2.35	1.35	1.32
9	A2	4272	OMU	O2-C2	-2.34	1.18	1.23
9	A2	2156	A2M	C2-N3	2.33	1.35	1.32
46	m2	1245	PSU	C1'-C5	2.32	1.55	1.50
9	A2	3523	A2M	C2-N3	2.32	1.35	1.32
9	A2	3958	OMU	O2-C2	-2.31	1.18	1.23
11	C2	14	OMU	O2-C2	-2.31	1.18	1.23
9	A2	1418	G7M	O6-C6	-2.30	1.18	1.23
9	A2	1685	OMG	O6-C6	-2.30	1.18	1.23
9	A2	4023	MHG	O6-C6	-2.30	1.19	1.23
9	A2	3958	OMU	C5-C4	2.29	1.48	1.43
9	A2	3441	A2M	C5-C4	-2.28	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	m2	116	OMU	C5-C4	2.28	1.48	1.43
9	A2	4280	PSU	C1'-C5	2.28	1.55	1.50
46	m2	614	PSU	C1'-C5	2.28	1.55	1.50
9	A2	4146	OMG	O6-C6	-2.27	1.18	1.23
46	m2	116	OMU	O2-C2	-2.27	1.18	1.23
9	A2	1395	PSU	C1'-C5	2.27	1.55	1.50
9	A2	1852	OMG	O6-C6	-2.27	1.18	1.23
9	A2	3385	PSU	C1'-C5	2.25	1.55	1.50
9	A2	4055	PSU	C1'-C5	2.25	1.55	1.50
9	A2	4515	OMG	O6-C6	-2.24	1.18	1.23
9	A2	4275	OMG	O6-C6	-2.23	1.18	1.23
9	A2	3837	B8W	O5'-C5'	-2.23	1.39	1.44
9	A2	4288	PSU	C1'-C5	2.22	1.55	1.50
9	A2	1673	A2M	C5-C4	-2.22	1.35	1.40
9	A2	2179	OMG	O6-C6	-2.22	1.18	1.23
9	A2	2119	OMG	O6-C6	-2.22	1.18	1.23
9	A2	2120	OMC	C5-C4	2.22	1.48	1.42
9	A2	373	OMG	O6-C6	-2.21	1.18	1.23
9	A2	878	2MG	O6-C6	-2.21	1.18	1.23
9	A2	1335	OMG	O6-C6	-2.21	1.18	1.23
9	A2	2528	OMG	O6-C6	-2.21	1.18	1.23
9	A2	3448	OMG	O6-C6	-2.21	1.18	1.23
46	m2	1083	PSU	C1'-C5	2.21	1.55	1.50
9	A2	1490	PSU	C1'-C5	2.20	1.55	1.50
9	A2	1438	OMG	O6-C6	-2.19	1.18	1.23
9	A2	4022	OMG	O6-C6	-2.19	1.18	1.23
9	A2	1472	I4U	C3'-C4'	2.19	1.58	1.53
46	m2	825	PSU	C1'-C5	2.19	1.55	1.50
9	A2	1347	A2M	C5-C4	-2.19	1.35	1.40
9	A2	1496	PSU	C1'-C5	2.18	1.55	1.50
46	m2	646	OMG	O6-C6	-2.18	1.18	1.23
9	A2	3523	A2M	C5-C4	-2.18	1.35	1.40
9	A2	4152	PSU	C1'-C5	2.18	1.55	1.50
9	A2	1337	A2M	C5-C4	-2.18	1.35	1.40
9	A2	2156	A2M	C5-C4	-2.18	1.35	1.40
9	A2	4183	PSU	C1'-C5	2.17	1.55	1.50
9	A2	4272	OMU	C5-C4	2.17	1.48	1.43
9	A2	2118	A2M	C5-C4	-2.17	1.35	1.40
9	A2	3481	A2M	C5-C4	-2.17	1.35	1.40
9	A2	4223	A2M	C5-C4	-2.17	1.35	1.40
9	A2	1330	2MG	O6-C6	-2.17	1.18	1.23
9	A2	1140	A2M	C5-C4	-2.17	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A2	3848	OMG	O6-C6	-2.16	1.18	1.23
9	A2	4023	MHG	C5-C4	2.15	1.45	1.38
9	A2	4517	2MG	O6-C6	-2.14	1.18	1.23
46	m2	670	A2M	C5-C4	-2.14	1.35	1.40
9	A2	398	A2M	C5-C4	-2.14	1.35	1.40
46	m2	1033	A2M	C5-C4	-2.14	1.35	1.40
9	A2	3872	6MZ	C2-N3	2.13	1.35	1.32
46	m2	27	A2M	C5-C4	-2.13	1.35	1.40
9	A2	3945	PSU	C1'-C5	2.13	1.55	1.50
46	m2	685	OMG	O6-C6	-2.13	1.19	1.23
46	m2	166	A2M	C5-C4	-2.13	1.35	1.40
46	m2	1250	B8N	C1'-C5	2.12	1.55	1.50
9	A2	3379	A2M	C5-C4	-2.12	1.35	1.40
9	A2	2118	A2M	C4-N3	-2.11	1.32	1.35
46	m2	1250	B8N	O4'-C1'	-2.11	1.40	1.43
9	A2	3374	A2M	C5-C4	-2.10	1.35	1.40
9	A2	3523	A2M	C4-N3	-2.07	1.32	1.35
46	m2	670	A2M	C4-N3	-2.04	1.32	1.35
9	A2	4102	PSU	C1'-C5	2.04	1.54	1.50
9	A2	1140	A2M	C4-N3	-2.04	1.32	1.35
9	A2	1347	A2M	C4-N3	-2.03	1.32	1.35
9	A2	4152	PSU	O4-C4	-2.02	1.19	1.23
9	A2	2541	B9H	O2-C2	-2.02	1.18	1.22
9	A2	4288	PSU	O4-C4	-2.02	1.19	1.23
9	A2	1395	PSU	O4-C4	-2.02	1.19	1.23
46	m2	27	A2M	C4-N3	-2.00	1.32	1.35
46	m2	825	PSU	O4-C4	-2.00	1.19	1.23

All (378) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	4023	MHG	C2-N3-C4	7.95	121.90	112.04
9	A2	3837	B8W	O6-C6-N1	7.88	129.96	119.03
9	A2	4183	PSU	N1-C2-N3	7.55	123.68	115.13
9	A2	3837	B8W	N2-C2-N3	7.54	130.08	117.79
9	A2	4152	PSU	N1-C2-N3	7.42	123.53	115.13
9	A2	1496	PSU	N1-C2-N3	7.39	123.50	115.13
9	A2	4055	PSU	N1-C2-N3	7.34	123.45	115.13
46	m2	825	PSU	N1-C2-N3	7.32	123.43	115.13
9	A2	3385	PSU	N1-C2-N3	7.32	123.42	115.13
9	A2	4094	PSU	N1-C2-N3	7.31	123.42	115.13
46	m2	1083	PSU	N1-C2-N3	7.29	123.39	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	3945	PSU	N1-C2-N3	7.29	123.39	115.13
9	A2	4280	PSU	N1-C2-N3	7.27	123.36	115.13
9	A2	1490	PSU	N1-C2-N3	7.27	123.36	115.13
9	A2	4102	PSU	N1-C2-N3	7.23	123.32	115.13
9	A2	4288	PSU	N1-C2-N3	7.22	123.31	115.13
9	A2	2263	PSU	N1-C2-N3	7.21	123.29	115.13
46	m2	614	PSU	N1-C2-N3	7.20	123.29	115.13
46	m2	1245	PSU	N1-C2-N3	7.19	123.27	115.13
9	A2	3371	PSU	N1-C2-N3	7.17	123.25	115.13
9	A2	1395	PSU	N1-C2-N3	7.15	123.23	115.13
9	A2	3420	PSU	N1-C2-N3	7.13	123.21	115.13
46	m2	824	PSU	N1-C2-N3	6.67	122.69	115.13
9	A2	3536	P7G	C4-C5-N7	6.34	110.01	106.67
9	A2	4023	MHG	C4-C5-N7	6.31	110.52	104.91
9	A2	1496	PSU	C4-N3-C2	-6.28	117.28	126.34
9	A2	4152	PSU	C4-N3-C2	-6.25	117.33	126.34
9	A2	1490	PSU	C4-N3-C2	-6.24	117.34	126.34
46	m2	825	PSU	C4-N3-C2	-6.21	117.39	126.34
9	A2	4055	PSU	C4-N3-C2	-6.21	117.40	126.34
9	A2	3945	PSU	C4-N3-C2	-6.19	117.43	126.34
9	A2	4183	PSU	C4-N3-C2	-6.16	117.46	126.34
9	A2	4288	PSU	C4-N3-C2	-6.16	117.46	126.34
9	A2	4102	PSU	C4-N3-C2	-6.16	117.47	126.34
46	m2	1083	PSU	C4-N3-C2	-6.14	117.49	126.34
46	m2	824	PSU	O2-C2-N1	-6.10	116.08	122.79
9	A2	3385	PSU	C4-N3-C2	-6.09	117.56	126.34
9	A2	4280	PSU	C4-N3-C2	-6.08	117.58	126.34
9	A2	1395	PSU	C4-N3-C2	-6.02	117.67	126.34
9	A2	2263	PSU	C4-N3-C2	-6.01	117.67	126.34
9	A2	4094	PSU	C4-N3-C2	-5.99	117.70	126.34
46	m2	1245	PSU	C4-N3-C2	-5.88	117.87	126.34
9	A2	3371	PSU	C4-N3-C2	-5.87	117.88	126.34
46	m2	824	PSU	C4-N3-C2	-5.87	117.88	126.34
46	m2	614	PSU	C4-N3-C2	-5.87	117.89	126.34
9	A2	2052	E7G	C4-C5-N7	5.83	110.10	104.91
9	A2	1599	E7G	C4-C5-N7	5.76	110.03	104.91
9	A2	3420	PSU	C4-N3-C2	-5.72	118.10	126.34
9	A2	1711	P7G	C4-C5-N7	5.61	109.63	106.67
46	m2	1250	B8N	C4-N3-C2	-5.59	118.39	125.46
46	m2	166	A2M	N3-C2-N1	-5.58	119.95	128.68
9	A2	3441	A2M	N3-C2-N1	-5.57	119.97	128.68
9	A2	1140	A2M	N3-C2-N1	-5.55	120.00	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	4223	A2M	N3-C2-N1	-5.55	120.00	128.68
9	A2	1673	A2M	N3-C2-N1	-5.55	120.01	128.68
9	A2	2156	A2M	N3-C2-N1	-5.55	120.01	128.68
9	A2	398	A2M	N3-C2-N1	-5.54	120.01	128.68
9	A2	3374	A2M	N3-C2-N1	-5.53	120.03	128.68
9	A2	3481	A2M	N3-C2-N1	-5.52	120.05	128.68
9	A2	3872	6MZ	N3-C2-N1	-5.51	120.06	128.68
46	m2	27	A2M	N3-C2-N1	-5.50	120.08	128.68
9	A2	1337	A2M	N3-C2-N1	-5.49	120.10	128.68
9	A2	1599	E7G	C2-N3-C4	5.47	122.05	112.30
46	m2	1033	A2M	N3-C2-N1	-5.46	120.14	128.68
9	A2	3379	A2M	N3-C2-N1	-5.45	120.16	128.68
9	A2	1347	A2M	N3-C2-N1	-5.45	120.16	128.68
9	A2	4067	1MA	N1-C2-N3	-5.41	119.71	126.02
9	A2	4007	E6G	N3-C2-N1	-5.36	120.07	127.22
46	m2	670	A2M	N3-C2-N1	-5.35	120.32	128.68
11	C2	14	OMU	C4-N3-C2	-5.34	119.54	126.58
9	A2	4183	PSU	C6-N1-C2	-5.33	117.23	122.68
9	A2	2118	A2M	N3-C2-N1	-5.30	120.39	128.68
9	A2	3420	PSU	C6-N1-C2	-5.30	117.27	122.68
9	A2	2052	E7G	C2-N3-C4	5.30	121.74	112.30
9	A2	3371	PSU	C6-N1-C2	-5.28	117.28	122.68
9	A2	4094	PSU	C6-N1-C2	-5.27	117.29	122.68
9	A2	1387	B9B	N3-C2-N1	-5.27	120.20	127.22
46	m2	614	PSU	C6-N1-C2	-5.23	117.33	122.68
9	A2	3958	OMU	C4-N3-C2	-5.23	119.68	126.58
9	A2	1269	B8Q	C31-N3-C4	5.23	122.13	114.25
46	m2	1245	PSU	C6-N1-C2	-5.22	117.34	122.68
9	A2	3523	A2M	N3-C2-N1	-5.22	120.52	128.68
9	A2	237	B9B	N3-C2-N1	-5.22	120.26	127.22
9	A2	3837	B8W	N3-C2-N1	-5.21	120.27	127.22
9	A2	4280	PSU	C6-N1-C2	-5.13	117.43	122.68
9	A2	3385	PSU	C6-N1-C2	-5.09	117.48	122.68
9	A2	3945	PSU	C6-N1-C2	-5.04	117.53	122.68
9	A2	4152	PSU	C6-N1-C2	-5.03	117.54	122.68
46	m2	825	PSU	C6-N1-C2	-5.00	117.57	122.68
9	A2	4055	PSU	C6-N1-C2	-5.00	117.57	122.68
9	A2	2263	PSU	C6-N1-C2	-5.00	117.57	122.68
9	A2	1395	PSU	C6-N1-C2	-4.99	117.58	122.68
9	A2	4023	MHG	C2-N1-C6	-4.98	118.75	124.48
9	A2	1496	PSU	C6-N1-C2	-4.98	117.59	122.68
46	m2	1250	B8N	C5-C4-N3	4.98	125.39	116.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	4102	PSU	C6-N1-C2	-4.96	117.61	122.68
9	A2	4288	PSU	C6-N1-C2	-4.96	117.61	122.68
46	m2	1083	PSU	C6-N1-C2	-4.95	117.62	122.68
9	A2	1490	PSU	C6-N1-C2	-4.89	117.68	122.68
9	A2	3837	B8W	N2-C2-N1	-4.89	109.65	117.25
46	m2	116	OMU	C4-N3-C2	-4.84	120.20	126.58
46	m2	1832	UR3	C4-N3-C2	-4.82	120.02	124.56
9	A2	4272	OMU	C4-N3-C2	-4.75	120.31	126.58
46	m2	824	PSU	C6-N1-C2	-4.71	117.86	122.68
9	A2	1269	B8Q	N3-C2-N1	4.66	122.61	117.13
79	m	714	DDE	CBW-CBI-NAD	4.58	121.11	115.28
9	A2	2541	B9H	C31-N3-C2	4.57	122.92	117.21
9	A2	4102	PSU	C6-C5-C4	4.54	121.37	118.20
9	A2	1668	UR3	C4-N3-C2	-4.52	120.30	124.56
9	A2	4152	PSU	C6-C5-C4	4.47	121.32	118.20
9	A2	4249	UR3	C4-N3-C2	-4.45	120.37	124.56
9	A2	1490	PSU	C6-C5-C4	4.42	121.29	118.20
9	A2	4183	PSU	C6-C5-C4	4.40	121.28	118.20
9	A2	1599	E7G	C5-C6-N1	4.39	118.73	110.99
46	m2	825	PSU	C6-C5-C4	4.34	121.23	118.20
9	A2	1496	PSU	C6-C5-C4	4.33	121.23	118.20
9	A2	3945	PSU	C6-C5-C4	4.31	121.21	118.20
9	A2	3837	B8W	C2-N3-C4	4.31	120.27	115.36
9	A2	4023	MHG	C5-C6-N1	4.30	118.57	110.99
46	m2	1083	PSU	C6-C5-C4	4.29	121.20	118.20
9	A2	4183	PSU	O2-C2-N1	-4.27	118.09	122.79
46	m2	614	PSU	O2-C2-N1	-4.26	118.10	122.79
9	A2	237	B9B	C2-N3-C4	4.25	120.21	115.36
9	A2	3385	PSU	O2-C2-N1	-4.24	118.13	122.79
9	A2	3385	PSU	C6-C5-C4	4.23	121.16	118.20
9	A2	2052	E7G	C5-C6-N1	4.21	118.42	110.99
9	A2	4007	E6G	C2-N3-C4	4.19	120.14	115.36
9	A2	4152	PSU	O2-C2-N1	-4.19	118.18	122.79
9	A2	4094	PSU	O2-C2-N1	-4.19	118.18	122.79
9	A2	4280	PSU	O2-C2-N1	-4.18	118.19	122.79
9	A2	1496	PSU	O2-C2-N1	-4.15	118.22	122.79
9	A2	3371	PSU	O2-C2-N1	-4.15	118.22	122.79
9	A2	1387	B9B	C2-N3-C4	4.14	120.09	115.36
9	A2	3837	B8W	O6-C6-C5	-4.11	110.13	116.01
9	A2	4288	PSU	O2-C2-N1	-4.11	118.26	122.79
46	m2	825	PSU	O2-C2-N1	-4.09	118.29	122.79
9	A2	4055	PSU	O2-C2-N1	-4.08	118.29	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	3420	PSU	O2-C2-N1	-4.08	118.29	122.79
9	A2	3945	PSU	O2-C2-N1	-4.08	118.30	122.79
46	m2	1245	PSU	C6-C5-C4	4.08	121.05	118.20
9	A2	4288	PSU	C6-C5-C4	4.07	121.04	118.20
9	A2	1395	PSU	O2-C2-N1	-4.06	118.31	122.79
46	m2	1083	PSU	O2-C2-N1	-4.06	118.32	122.79
9	A2	4055	PSU	C6-C5-C4	4.05	121.03	118.20
9	A2	1490	PSU	O2-C2-N1	-4.04	118.34	122.79
9	A2	4280	PSU	C6-C5-C4	4.02	121.01	118.20
9	A2	4102	PSU	O2-C2-N1	-4.02	118.37	122.79
9	A2	3872	6MZ	C2-N1-C6	3.98	120.01	116.59
9	A2	2263	PSU	O2-C2-N1	-3.98	118.41	122.79
9	A2	1395	PSU	C6-C5-C4	3.97	120.97	118.20
9	A2	4007	E6G	C61-O6-C6	-3.96	113.64	117.56
46	m2	1245	PSU	O2-C2-N1	-3.95	118.44	122.79
9	A2	4272	OMU	N3-C2-N1	3.89	120.06	114.89
9	A2	4023	MHG	C5-C4-N3	-3.86	120.78	128.13
46	m2	614	PSU	C6-C5-C4	3.86	120.89	118.20
9	A2	4094	PSU	C6-C5-C4	3.80	120.85	118.20
11	C2	14	OMU	N3-C2-N1	3.75	119.87	114.89
9	A2	1140	A2M	C5-C6-N6	3.75	126.05	120.35
9	A2	237	B9B	C3'-C2'-C1'	3.71	106.56	100.98
9	A2	3958	OMU	N3-C2-N1	3.68	119.78	114.89
9	A2	1418	G7M	C2-N1-C6	-3.68	118.32	125.10
9	A2	2277	G7M	C2-N1-C6	-3.67	118.34	125.10
9	A2	3371	PSU	C6-C5-C4	3.66	120.75	118.20
46	m2	166	A2M	C5-C6-N6	3.65	125.89	120.35
46	m2	1033	A2M	C5-C6-N6	3.64	125.89	120.35
9	A2	2118	A2M	C5-C6-N6	3.62	125.86	120.35
9	A2	3379	A2M	C5-C6-N6	3.62	125.86	120.35
9	A2	3523	A2M	C5-C6-N6	3.62	125.85	120.35
9	A2	4223	A2M	C5-C6-N6	3.62	125.85	120.35
9	A2	1599	E7G	C2-N1-C6	-3.62	118.50	125.10
46	m2	670	A2M	C5-C6-N6	3.61	125.84	120.35
9	A2	1599	E7G	C5-C4-N3	-3.60	121.26	128.13
9	A2	1347	A2M	C5-C6-N6	3.59	125.80	120.35
9	A2	3481	A2M	C5-C6-N6	3.58	125.80	120.35
9	A2	4202	G7M	C2-N1-C6	-3.58	118.50	125.10
46	m2	116	OMU	N3-C2-N1	3.58	119.64	114.89
9	A2	398	A2M	C5-C6-N6	3.57	125.78	120.35
9	A2	2263	PSU	C6-C5-C4	3.56	120.69	118.20
9	A2	1337	A2M	C5-C6-N6	3.54	125.73	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	1673	A2M	C5-C6-N6	3.54	125.73	120.35
9	A2	1685	OMG	C5-C6-N1	3.51	120.15	113.95
46	m2	824	PSU	C6-C5-C4	3.50	120.64	118.20
9	A2	3374	A2M	C5-C6-N6	3.49	125.66	120.35
9	A2	2528	OMG	C5-C6-N1	3.48	120.10	113.95
9	A2	1335	OMG	C5-C6-N1	3.48	120.10	113.95
9	A2	2052	E7G	C5-C4-N3	-3.47	121.51	128.13
9	A2	2156	A2M	C5-C6-N6	3.47	125.63	120.35
9	A2	4022	OMG	C5-C6-N1	3.47	120.08	113.95
9	A2	4275	OMG	C5-C6-N1	3.47	120.08	113.95
9	A2	878	2MG	C5-C6-N1	3.47	120.07	113.95
9	A2	1472	I4U	C5-C4-N3	-3.46	119.64	124.91
9	A2	4146	OMG	C5-C6-N1	3.46	120.06	113.95
9	A2	3448	OMG	C5-C6-N1	3.44	120.03	113.95
9	A2	1438	OMG	C5-C6-N1	3.44	120.02	113.95
9	A2	2119	OMG	C5-C6-N1	3.43	120.01	113.95
9	A2	2052	E7G	C2-N1-C6	-3.42	118.86	125.10
11	C2	14	OMU	C5-C4-N3	3.42	119.95	114.84
9	A2	1330	2MG	C5-C6-N1	3.41	119.98	113.95
9	A2	2179	OMG	C5-C6-N1	3.41	119.97	113.95
9	A2	1852	OMG	C5-C6-N1	3.40	119.96	113.95
46	m2	646	OMG	C5-C6-N1	3.40	119.95	113.95
9	A2	3958	OMU	C5-C4-N3	3.38	119.90	114.84
9	A2	3846	I4U	C5-C4-N3	-3.37	119.78	124.91
9	A2	3987	5MC	C5-C6-N1	-3.37	119.87	123.34
9	A2	3848	OMG	C5-C6-N1	3.37	119.91	113.95
9	A2	3420	PSU	C6-C5-C4	3.36	120.55	118.20
46	m2	685	OMG	C5-C6-N1	3.36	119.88	113.95
9	A2	4515	OMG	C5-C6-N1	3.35	119.86	113.95
9	A2	4289	OMG	C5-C6-N1	3.34	119.85	113.95
9	A2	373	OMG	C5-C6-N1	3.32	119.82	113.95
9	A2	4517	2MG	C5-C6-N1	3.32	119.81	113.95
46	m2	27	A2M	C5-C6-N6	3.28	125.34	120.35
9	A2	3441	A2M	C1'-N9-C4	-3.25	120.93	126.64
9	A2	4099	5MC	C5-C6-N1	-3.24	120.00	123.34
46	m2	1250	B8N	O4-C4-N3	-3.24	114.48	119.98
9	A2	4023	MHG	C72-C71-N7	-3.24	109.22	112.41
9	A2	3441	A2M	C5-C6-N6	3.23	125.25	120.35
9	A2	3438	5MC	C5-C6-N1	-3.22	120.03	123.34
9	A2	4067	1MA	C5-C6-N1	3.19	118.65	113.90
9	A2	3523	A2M	C1'-N9-C4	-3.18	121.06	126.64
46	m2	116	OMU	C5-C4-N3	3.15	119.55	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	4007	E6G	N2-C2-N3	3.11	122.86	117.79
9	A2	3481	A2M	C1'-N9-C4	-3.10	121.19	126.64
9	A2	4223	A2M	C1'-N9-C4	-3.07	121.25	126.64
9	A2	4289	OMG	C8-N7-C5	3.06	108.82	102.99
9	A2	1438	OMG	C2-N1-C6	-3.04	119.49	125.10
46	m2	1844	4AC	C6-C5-C4	3.03	120.67	116.96
9	A2	1140	A2M	C1'-N9-C4	-3.01	121.35	126.64
9	A2	1269	B8Q	O2-C2-N3	-3.01	118.53	122.95
9	A2	1269	B8Q	C6-N1-C2	-3.00	119.10	121.79
9	A2	4272	OMU	C5-C4-N3	3.00	119.33	114.84
9	A2	1269	B8Q	C31-N3-C2	3.00	122.15	117.79
9	A2	398	A2M	C1'-N9-C4	-3.00	121.37	126.64
9	A2	4289	OMG	C2-N1-C6	-2.99	119.58	125.10
9	A2	3448	OMG	C2-N1-C6	-2.98	119.61	125.10
9	A2	1852	OMG	C2-N1-C6	-2.98	119.62	125.10
9	A2	2528	OMG	C2-N1-C6	-2.97	119.62	125.10
9	A2	4275	OMG	C2-N1-C6	-2.97	119.62	125.10
9	A2	1335	OMG	C2-N1-C6	-2.97	119.63	125.10
9	A2	1335	OMG	C8-N7-C5	2.95	108.61	102.99
9	A2	1685	OMG	C2-N1-C6	-2.95	119.67	125.10
9	A2	2119	OMG	C2-N1-C6	-2.94	119.68	125.10
9	A2	4146	OMG	C2-N1-C6	-2.94	119.69	125.10
9	A2	4022	OMG	C2-N1-C6	-2.93	119.69	125.10
9	A2	1673	A2M	C1'-N9-C4	-2.93	121.49	126.64
46	m2	646	OMG	C8-N7-C5	2.93	108.57	102.99
46	m2	646	OMG	C2-N1-C6	-2.93	119.70	125.10
9	A2	4275	OMG	C8-N7-C5	2.93	108.57	102.99
9	A2	2052	E7G	C5-C4-N9	2.93	110.14	106.35
9	A2	3448	OMG	C8-N7-C5	2.93	108.56	102.99
9	A2	2156	A2M	C1'-N9-C4	-2.92	121.51	126.64
46	m2	685	OMG	C8-N7-C5	2.92	108.55	102.99
9	A2	4515	OMG	C2-N1-C6	-2.91	119.74	125.10
9	A2	3379	A2M	C1'-N9-C4	-2.91	121.53	126.64
9	A2	3958	OMU	O4-C4-C5	-2.90	120.06	125.16
9	A2	3848	OMG	C8-N7-C5	2.89	108.50	102.99
9	A2	2179	OMG	C2-N1-C6	-2.89	119.78	125.10
9	A2	3848	OMG	C2-N1-C6	-2.88	119.79	125.10
9	A2	4146	OMG	C8-N7-C5	2.88	108.48	102.99
46	m2	685	OMG	C2-N1-C6	-2.88	119.80	125.10
9	A2	4515	OMG	C8-N7-C5	2.87	108.46	102.99
9	A2	373	OMG	C8-N7-C5	2.87	108.45	102.99
9	A2	4023	MHG	N9-C4-N3	2.86	129.75	125.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	2119	OMG	C8-N7-C5	2.85	108.43	102.99
9	A2	4022	OMG	C8-N7-C5	2.85	108.42	102.99
46	m2	166	A2M	C1'-N9-C4	-2.85	121.63	126.64
46	m2	27	A2M	C1'-N9-C4	-2.85	121.64	126.64
9	A2	1438	OMG	C8-N7-C5	2.84	108.40	102.99
9	A2	1685	OMG	C8-N7-C5	2.84	108.39	102.99
9	A2	1599	E7G	C5-C4-N9	2.82	110.01	106.35
9	A2	373	OMG	C2-N1-C6	-2.81	119.92	125.10
46	m2	116	OMU	O4-C4-C5	-2.81	120.22	125.16
9	A2	1852	OMG	C8-N7-C5	2.81	108.34	102.99
9	A2	2179	OMG	C8-N7-C5	2.80	108.32	102.99
9	A2	2528	OMG	C8-N7-C5	2.76	108.25	102.99
9	A2	4272	OMU	O4-C4-C5	-2.76	120.31	125.16
11	C2	14	OMU	O4-C4-C5	-2.73	120.35	125.16
9	A2	1668	UR3	C1'-N1-C2	2.73	121.59	116.99
9	A2	2541	B9H	O3'-C3'-C2'	2.71	118.87	111.17
9	A2	2541	B9H	C6-N1-C2	-2.71	119.36	121.79
9	A2	4067	1MA	C8-N7-C5	2.69	108.11	102.99
46	m2	670	A2M	C1'-N9-C4	-2.68	121.93	126.64
46	m2	1033	A2M	C1'-N9-C4	-2.64	122.00	126.64
9	A2	237	B9B	N2-C2-N3	2.64	122.09	117.79
9	A2	2177	OMC	C1'-N1-C6	2.63	126.58	120.84
9	A2	2118	A2M	C1'-N9-C4	-2.63	122.02	126.64
9	A2	1472	I4U	C3'-C2'-C1'	2.60	106.37	101.43
9	A2	1668	UR3	C6-N1-C2	-2.60	119.46	121.79
9	A2	4517	2MG	C8-N7-C5	2.60	107.94	102.99
9	A2	1330	2MG	C8-N7-C5	2.59	107.93	102.99
9	A2	1347	A2M	C1'-N9-C4	-2.59	122.09	126.64
9	A2	3374	A2M	C1'-N9-C4	-2.57	122.12	126.64
9	A2	1599	E7G	O6-C6-C5	-2.56	121.25	127.54
9	A2	1387	B9B	N2-C2-N3	2.56	121.97	117.79
9	A2	1387	B9B	C3'-C2'-C1'	2.56	104.83	100.98
9	A2	2052	E7G	C8-N7-C71	2.52	126.50	120.50
9	A2	878	2MG	C8-N7-C5	2.50	107.75	102.99
9	A2	2528	OMG	O6-C6-C5	-2.50	119.50	124.37
9	A2	4023	MHG	N1-C2-N3	-2.48	120.12	123.95
9	A2	2052	E7G	N9-C8-N7	2.46	106.89	103.38
46	m2	1250	B8N	C31-N3-C4	2.45	120.93	117.31
9	A2	1337	A2M	C1'-N9-C4	-2.45	122.33	126.64
9	A2	1685	OMG	O6-C6-C5	-2.45	119.59	124.37
9	A2	4023	MHG	N9-C8-N7	2.41	106.83	103.38
9	A2	4023	MHG	C5-C4-N9	2.41	109.48	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A2	4515	OMG	O6-C6-C5	-2.41	119.67	124.37
9	A2	3837	B8W	C2-N1-C6	2.41	119.95	116.08
9	A2	2052	E7G	O6-C6-C5	-2.40	121.65	127.54
9	A2	4007	E6G	C2-N1-C6	2.40	119.94	116.08
9	A2	4249	UR3	C6-N1-C2	-2.39	119.65	121.79
9	A2	2541	B9H	O2-C2-N3	-2.39	119.04	122.07
9	A2	4023	MHG	C21-N2-C2	-2.39	118.59	123.86
9	A2	4135	B8T	C6-C5-C4	2.37	119.86	116.96
9	A2	3837	B8W	C1'-N9-C4	-2.35	122.51	126.64
9	A2	1599	E7G	N9-C8-N7	2.35	106.74	103.38
9	A2	237	B9B	C2-N1-C6	2.35	119.85	116.08
46	m2	1844	4AC	C5-C4-N3	-2.34	118.82	122.59
46	m2	1844	4AC	N4-C4-N3	2.33	117.76	113.85
9	A2	4023	MHG	O6-C6-C5	-2.32	121.84	127.54
9	A2	2179	OMG	O6-C6-C5	-2.32	119.84	124.37
9	A2	2119	OMG	O6-C6-C5	-2.31	119.86	124.37
9	A2	3536	P7G	N9-C8-N7	2.31	106.68	103.38
9	A2	878	2MG	O6-C6-C5	-2.31	119.87	124.37
9	A2	1387	B9B	O6-C6-N1	-2.30	118.14	120.12
9	A2	1711	P7G	N9-C8-N7	2.28	106.64	103.38
9	A2	4249	UR3	C1'-N1-C2	2.28	120.83	116.99
9	A2	4275	OMG	O6-C6-C5	-2.27	119.93	124.37
9	A2	4517	2MG	CM2-N2-C2	-2.27	118.84	123.86
9	A2	1335	OMG	O6-C6-C5	-2.27	119.94	124.37
9	A2	1387	B9B	C2-N1-C6	2.27	119.72	116.08
9	A2	373	OMG	O6-C6-C5	-2.26	119.95	124.37
9	A2	1330	2MG	O6-C6-C5	-2.26	119.95	124.37
46	m2	685	OMG	O6-C6-C5	-2.26	119.96	124.37
46	m2	646	OMG	O6-C6-C5	-2.26	119.97	124.37
9	A2	3848	OMG	O6-C6-C5	-2.25	119.97	124.37
9	A2	3448	OMG	O6-C6-C5	-2.25	119.97	124.37
9	A2	2120	OMC	O2-C2-N3	-2.25	118.67	122.33
9	A2	1438	OMG	O6-C6-C5	-2.24	120.00	124.37
9	A2	1599	E7G	C8-N7-C71	2.24	125.83	120.50
9	A2	4007	E6G	C3'-C2'-C1'	2.22	104.32	100.98
9	A2	4022	OMG	O6-C6-C5	-2.22	120.03	124.37
9	A2	2120	OMC	O2-C2-N1	2.22	123.47	118.89
9	A2	3837	B8W	C3'-C2'-C1'	2.22	104.32	100.98
9	A2	4146	OMG	O6-C6-C5	-2.21	120.05	124.37
9	A2	4517	2MG	O6-C6-C5	-2.21	120.06	124.37
9	A2	2616	OMC	O2-C2-N3	-2.19	118.76	122.33
9	A2	1140	A2M	N6-C6-N1	-2.19	114.02	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	m	714	DDE	OAG-CBI-NAD	-2.19	119.19	123.00
9	A2	1852	OMG	O6-C6-C5	-2.19	120.10	124.37
9	A2	3958	OMU	O2-C2-N1	-2.18	119.88	122.79
9	A2	1599	E7G	N9-C4-N3	2.18	128.73	125.47
9	A2	3987	5MC	CM5-C5-C6	-2.13	120.01	122.85
46	m2	166	A2M	N6-C6-N1	-2.13	114.16	118.57
46	m2	670	A2M	N6-C6-N1	-2.12	114.17	118.57
9	A2	3379	A2M	N6-C6-N1	-2.12	114.18	118.57
9	A2	3371	PSU	O4'-C1'-C2'	2.11	108.12	105.14
9	A2	3523	A2M	N6-C6-N1	-2.11	114.19	118.57
9	A2	3481	A2M	N6-C6-N1	-2.11	114.20	118.57
9	A2	1337	A2M	N6-C6-N1	-2.11	114.20	118.57
46	m2	1033	A2M	N6-C6-N1	-2.10	114.21	118.57
9	A2	1347	A2M	N6-C6-N1	-2.10	114.22	118.57
9	A2	2118	A2M	N6-C6-N1	-2.10	114.22	118.57
9	A2	1673	A2M	N6-C6-N1	-2.09	114.23	118.57
9	A2	4223	A2M	N6-C6-N1	-2.09	114.24	118.57
46	m2	1250	B8N	O4'-C1'-C2'	2.08	108.08	105.14
9	A2	2120	OMC	C1'-N1-C2	2.08	123.06	118.42
46	m2	1832	UR3	C6-N1-C2	-2.07	119.94	121.79
46	m2	614	PSU	O4'-C1'-C2'	2.06	108.05	105.14
9	A2	2156	A2M	N6-C6-N1	-2.05	114.31	118.57
9	A2	3374	A2M	N6-C6-N1	-2.04	114.33	118.57
9	A2	398	A2M	N6-C6-N1	-2.04	114.33	118.57
9	A2	4055	PSU	O4'-C1'-C2'	2.04	108.02	105.14
9	A2	1269	B8Q	C1'-N1-C2	2.03	120.42	116.99
46	m2	519	OMC	O2-C2-N3	-2.03	119.03	122.33
9	A2	1490	PSU	O4'-C1'-C2'	2.01	107.98	105.14
46	m2	1250	B8N	C31-N3-C2	2.01	120.69	117.67
9	A2	4094	PSU	O4'-C1'-C2'	2.00	107.97	105.14
9	A2	1330	2MG	CM2-N2-C2	-2.00	119.44	123.86

There are no chirality outliers.

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	g2	98	MLZ	C-CA-CB-CG
79	m	714	DDE	O-C-CA-CB
79	m	714	DDE	CA-CB-CG-ND1
79	m	714	DDE	NAD-CBI-CBW-NCB
79	m	714	DDE	CAT-CAU-CBW-CBI
79	m	714	DDE	CAT-CAU-CBW-NCB

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Mol	Chain	Res	Type	Atoms
9	A2	237	B9B	C5-C6-O6-C61
9	A2	237	B9B	N1-C6-O6-C61
9	A2	237	B9B	C3'-C4'-C5'-O5'
9	A2	237	B9B	C4'-C5'-O5'-P
9	A2	237	B9B	C62-C61-O6-C6
9	A2	398	A2M	C1'-C2'-O2'-CM'
9	A2	878	2MG	O4'-C4'-C5'-O5'
9	A2	878	2MG	C3'-C4'-C5'-O5'
9	A2	1140	A2M	C1'-C2'-O2'-CM'
9	A2	1387	B9B	C5-C6-O6-C61
9	A2	1387	B9B	N1-C6-O6-C61
9	A2	1395	PSU	C3'-C4'-C5'-O5'
9	A2	1395	PSU	O4'-C4'-C5'-O5'
9	A2	1490	PSU	C2'-C1'-C5-C4
9	A2	1668	UR3	O4'-C4'-C5'-O5'
9	A2	1668	UR3	C3'-C4'-C5'-O5'
9	A2	1685	OMG	O4'-C4'-C5'-O5'
9	A2	1685	OMG	C3'-C4'-C5'-O5'
9	A2	2052	E7G	C72-C71-N7-C5
9	A2	2119	OMG	O4'-C4'-C5'-O5'
9	A2	2119	OMG	C3'-C4'-C5'-O5'
9	A2	2156	A2M	O4'-C4'-C5'-O5'
9	A2	2156	A2M	C3'-C4'-C5'-O5'
9	A2	2177	OMC	C1'-C2'-O2'-CM2
9	A2	2528	OMG	C3'-C4'-C5'-O5'
9	A2	3374	A2M	C1'-C2'-O2'-CM'
9	A2	3379	A2M	C1'-C2'-O2'-CM'
9	A2	3385	PSU	O4'-C4'-C5'-O5'
9	A2	3420	PSU	C3'-C4'-C5'-O5'
9	A2	3420	PSU	O4'-C4'-C5'-O5'
9	A2	3438	5MC	O4'-C4'-C5'-O5'
9	A2	3481	A2M	C1'-C2'-O2'-CM'
9	A2	3523	A2M	O4'-C4'-C5'-O5'
9	A2	3523	A2M	C3'-C4'-C5'-O5'
9	A2	3523	A2M	C1'-C2'-O2'-CM'
9	A2	3536	P7G	C3'-C4'-C5'-O5'
9	A2	3536	P7G	O4'-C4'-C5'-O5'
9	A2	3543	OMC	C3'-C4'-C5'-O5'
9	A2	3837	B8W	C5-C6-O6-C61
9	A2	3837	B8W	N1-C6-O6-C61
9	A2	3846	I4U	O4'-C4'-C5'-O5'
9	A2	3872	6MZ	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
9	A2	3872	6MZ	N1-C6-N6-C9
9	A2	3958	OMU	C3'-C4'-C5'-O5'
9	A2	3958	OMU	O4'-C4'-C5'-O5'
9	A2	4007	E6G	C5-C6-O6-C61
9	A2	4007	E6G	N1-C6-O6-C61
9	A2	4023	MHG	C2'-C1'-N9-C8
9	A2	4099	5MC	C2'-C1'-N1-C2
9	A2	4099	5MC	C2'-C1'-N1-C6
9	A2	4183	PSU	O4'-C1'-C5-C6
9	A2	4223	A2M	C1'-C2'-O2'-CM'
9	A2	4272	OMU	C1'-C2'-O2'-CM2
9	A2	4288	PSU	C2'-C1'-C5-C4
9	A2	4288	PSU	C3'-C4'-C5'-O5'
9	A2	4288	PSU	O4'-C4'-C5'-O5'
9	A2	4515	OMG	C4'-C5'-O5'-P
46	m2	27	A2M	C1'-C2'-O2'-CM'
46	m2	116	OMU	C1'-C2'-O2'-CM2
46	m2	166	A2M	C3'-C4'-C5'-O5'
46	m2	519	OMC	O4'-C4'-C5'-O5'
46	m2	646	OMG	C1'-C2'-O2'-CM2
46	m2	685	OMG	O4'-C4'-C5'-O5'
46	m2	685	OMG	C3'-C4'-C5'-O5'
46	m2	824	PSU	C2'-C1'-C5-C6
46	m2	824	PSU	C3'-C4'-C5'-O5'
46	m2	824	PSU	O4'-C4'-C5'-O5'
46	m2	1250	B8N	O4'-C1'-C5-C6
46	m2	1250	B8N	O4'-C1'-C5-C4
46	m2	1250	B8N	N3-C31-C32-C33
11	C2	14	OMU	C4'-C5'-O5'-P
9	A2	237	B9B	O4'-C4'-C5'-O5'
9	A2	398	A2M	O4'-C4'-C5'-O5'
9	A2	1347	A2M	O4'-C4'-C5'-O5'
9	A2	1347	A2M	C3'-C4'-C5'-O5'
9	A2	3385	PSU	C3'-C4'-C5'-O5'
9	A2	3945	PSU	C3'-C4'-C5'-O5'
9	A2	4023	MHG	O4'-C4'-C5'-O5'
46	m2	166	A2M	O4'-C4'-C5'-O5'
46	m2	519	OMC	C3'-C4'-C5'-O5'
9	A2	398	A2M	C3'-C4'-C5'-O5'
9	A2	1438	OMG	O4'-C4'-C5'-O5'
9	A2	2528	OMG	O4'-C4'-C5'-O5'
9	A2	3438	5MC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
9	A2	3846	I4U	C3'-C4'-C5'-O5'
9	A2	3945	PSU	O4'-C4'-C5'-O5'
9	A2	4102	PSU	C3'-C4'-C5'-O5'
9	A2	4102	PSU	O4'-C4'-C5'-O5'
46	m2	1245	PSU	O4'-C4'-C5'-O5'
9	A2	4152	PSU	C3'-C4'-C5'-O5'
9	A2	3357	OMC	C2'-C1'-N1-C6
46	m2	1832	UR3	C2'-C1'-N1-C6
9	A2	1438	OMG	C3'-C4'-C5'-O5'
9	A2	3872	6MZ	C3'-C4'-C5'-O5'
46	m2	1245	PSU	C3'-C4'-C5'-O5'
9	A2	2052	E7G	C72-C71-N7-C8
9	A2	2179	OMG	O4'-C4'-C5'-O5'
9	A2	2179	OMG	C3'-C4'-C5'-O5'
9	A2	3543	OMC	O4'-C4'-C5'-O5'
9	A2	3872	6MZ	O4'-C4'-C5'-O5'
9	A2	4067	1MA	O4'-C4'-C5'-O5'
9	A2	4152	PSU	O4'-C4'-C5'-O5'
9	A2	3543	OMC	C4'-C5'-O5'-P
9	A2	3441	A2M	O4'-C4'-C5'-O5'
9	A2	4023	MHG	C3'-C4'-C5'-O5'
9	A2	4067	1MA	C3'-C4'-C5'-O5'
9	A2	1711	P7G	C72-C71-N7-C8
79	m	714	DDE	OAG-CBI-CBW-NCB
14	F2	333	MLZ	CD-CE-NZ-CM
9	A2	3441	A2M	C3'-C4'-C5'-O5'
9	A2	4007	E6G	O4'-C4'-C5'-O5'
79	m	714	DDE	CAU-CAT-CE1-ND1
46	m2	1033	A2M	C1'-C2'-O2'-CM'
9	A2	4099	5MC	O4'-C1'-N1-C6
46	m2	1832	UR3	C2'-C1'-N1-C2
9	A2	4099	5MC	O4'-C1'-N1-C2
46	m2	1832	UR3	O4'-C1'-N1-C6
9	A2	1438	OMG	C4'-C5'-O5'-P
9	A2	3987	5MC	C4'-C5'-O5'-P
46	m2	670	A2M	C4'-C5'-O5'-P
9	A2	3357	OMC	O4'-C1'-N1-C6
46	m2	166	A2M	C4'-C5'-O5'-P
9	A2	4289	OMG	C3'-C4'-C5'-O5'
9	A2	3357	OMC	C2'-C1'-N1-C2
9	A2	2179	OMG	C4'-C5'-O5'-P
9	A2	3958	OMU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
9	A2	4152	PSU	C4'-C5'-O5'-P
46	m2	1832	UR3	O4'-C1'-N1-C2
9	A2	2052	E7G	C3'-C4'-C5'-O5'
9	A2	4288	PSU	C4'-C5'-O5'-P
46	m2	519	OMC	C4'-C5'-O5'-P
9	A2	3357	OMC	C3'-C2'-O2'-CM2
46	m2	519	OMC	C3'-C2'-O2'-CM2
9	A2	373	OMG	C4'-C5'-O5'-P
9	A2	1387	B9B	C4'-C5'-O5'-P
9	A2	3357	OMC	O4'-C1'-N1-C2
46	m2	646	OMG	C4'-C5'-O5'-P
9	A2	1490	PSU	O4'-C1'-C5-C4
9	A2	4102	PSU	O4'-C1'-C5-C4
9	A2	4152	PSU	O4'-C1'-C5-C4
9	A2	4288	PSU	O4'-C1'-C5-C4
46	m2	1245	PSU	O4'-C1'-C5-C4
46	m2	1083	PSU	C4'-C5'-O5'-P
9	A2	1599	E7G	O4'-C4'-C5'-O5'
9	A2	3536	P7G	N7-C71-C72-C73
9	A2	2052	E7G	O4'-C4'-C5'-O5'
9	A2	4289	OMG	O4'-C4'-C5'-O5'
9	A2	2177	OMC	O4'-C1'-N1-C6
9	A2	4023	MHG	C2'-C1'-N9-C4
9	A2	2177	OMC	O4'-C1'-N1-C2
9	A2	1490	PSU	O4'-C1'-C5-C6
9	A2	4288	PSU	O4'-C1'-C5-C6
46	m2	1250	B8N	C31-C32-C33-N34
9	A2	3872	6MZ	C4'-C5'-O5'-P
9	A2	2177	OMC	O4'-C4'-C5'-O5'
9	A2	2177	OMC	C2'-C1'-N1-C6

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 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	GDP	m	900	-	24,30,30	3.45	14 (58%)	30,47,47	1.46	6 (20%)

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
88	GDP	m	900	-	-	5/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	m	900	GDP	O4'-C1'	7.73	1.51	1.41
88	m	900	GDP	O4'-C4'	-6.00	1.31	1.45
88	m	900	GDP	C2-N3	5.56	1.46	1.33
88	m	900	GDP	C3'-C4'	5.44	1.66	1.53
88	m	900	GDP	C4-N3	4.88	1.49	1.37
88	m	900	GDP	C2-N2	4.62	1.45	1.34
88	m	900	GDP	C2'-C1'	4.32	1.60	1.53
88	m	900	GDP	C6-N1	3.80	1.43	1.37
88	m	900	GDP	O2'-C2'	3.30	1.50	1.43
88	m	900	GDP	C5-C6	3.16	1.53	1.47
88	m	900	GDP	C2-N1	2.79	1.44	1.37
88	m	900	GDP	C5-C4	-2.52	1.36	1.43
88	m	900	GDP	O6-C6	-2.24	1.18	1.23
88	m	900	GDP	O3'-C3'	2.24	1.48	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	m	900	GDP	C5-C6-N1	3.37	119.90	113.95
88	m	900	GDP	C8-N7-C5	3.23	109.14	102.99
88	m	900	GDP	PA-O3A-PB	-2.98	122.59	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	m	900	GDP	C2-N1-C6	-2.85	119.85	125.10
88	m	900	GDP	O6-C6-C5	-2.24	120.00	124.37
88	m	900	GDP	O4'-C4'-C3'	2.19	109.45	105.11

There are no chirality outliers.

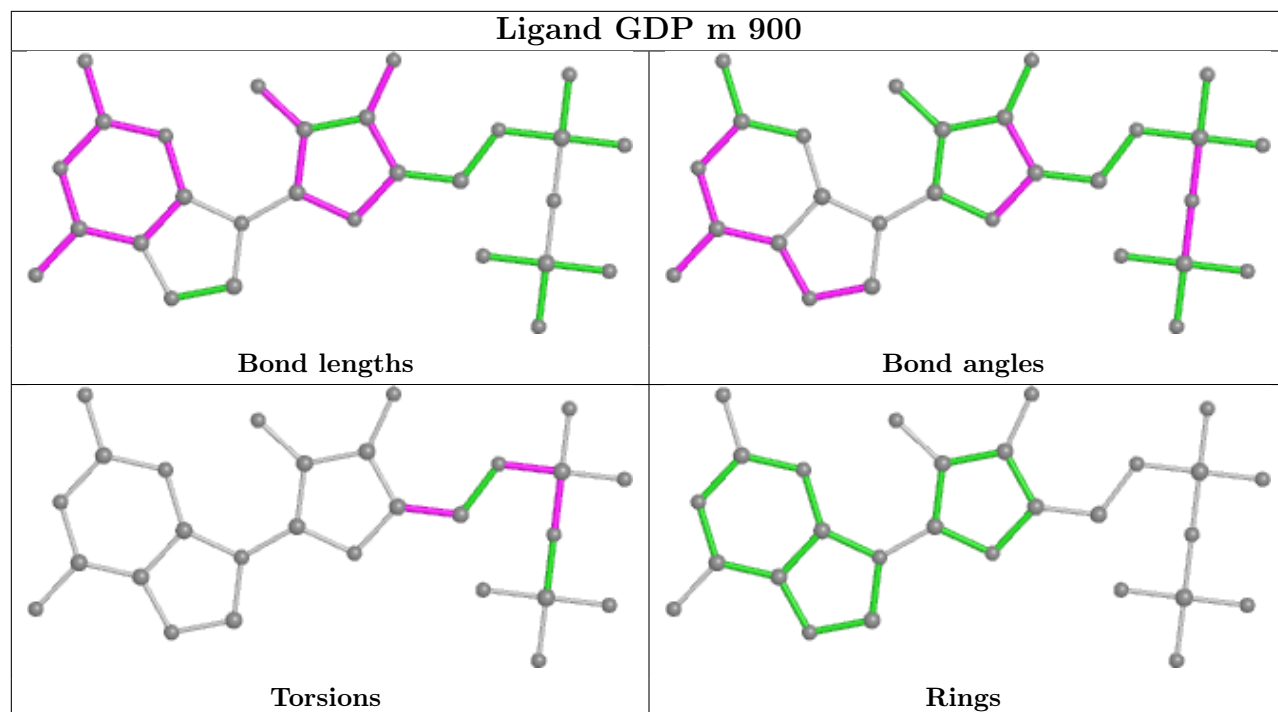
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	m	900	GDP	C5'-O5'-PA-O1A
88	m	900	GDP	C5'-O5'-PA-O2A
88	m	900	GDP	PB-O3A-PA-O2A
88	m	900	GDP	C5'-O5'-PA-O3A
88	m	900	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

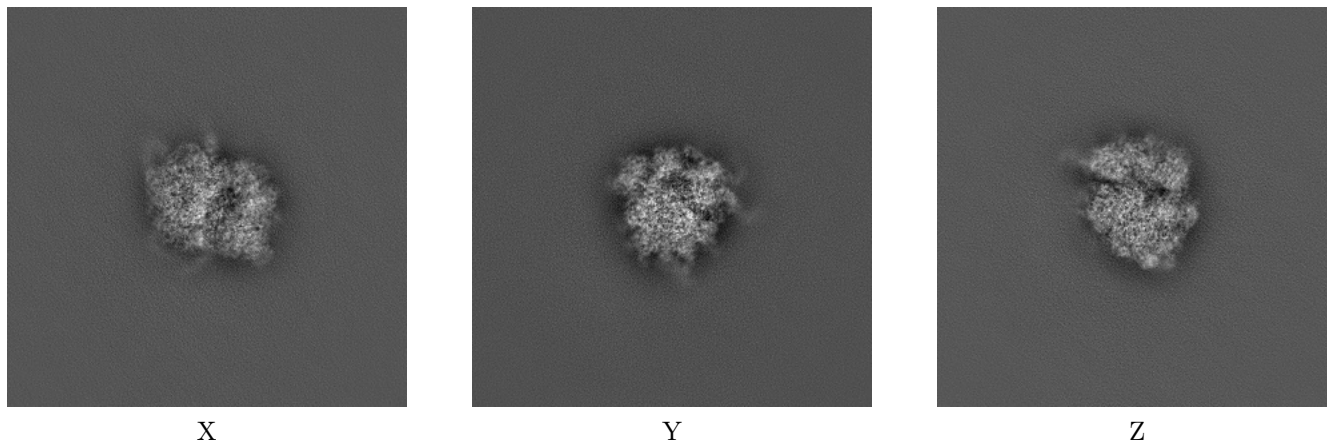
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23501. These allow visual inspection of the internal detail of the map and identification of artifacts.

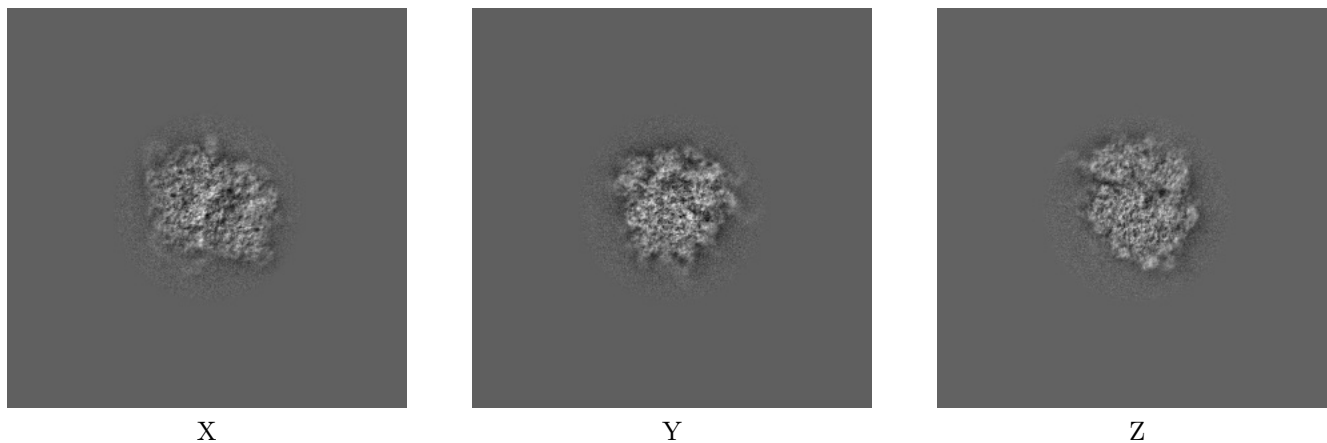
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



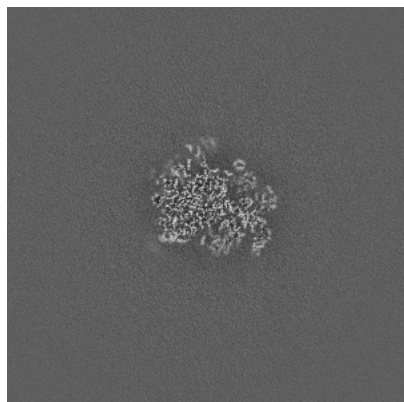
6.1.2 Raw map



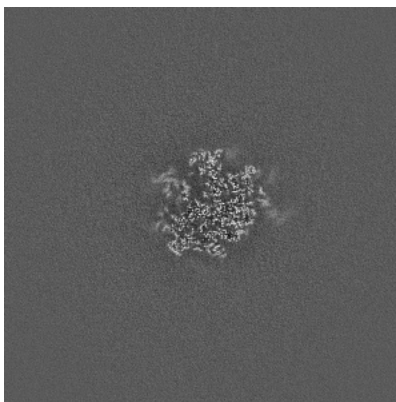
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

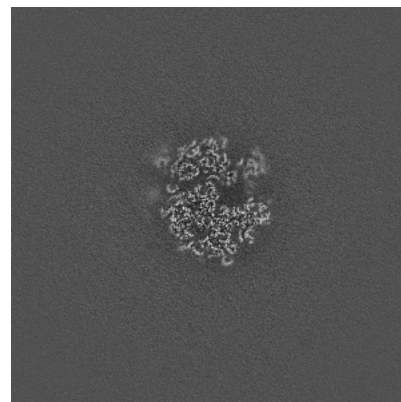
6.2.1 Primary map



X Index: 384

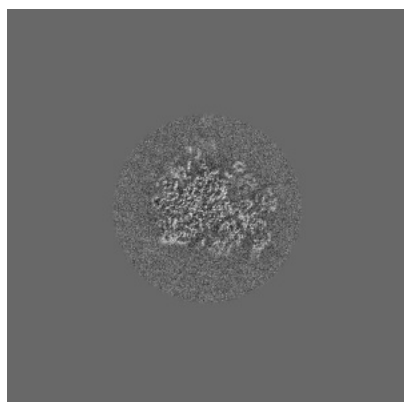


Y Index: 384

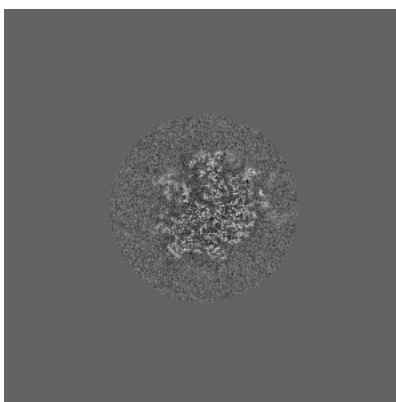


Z Index: 384

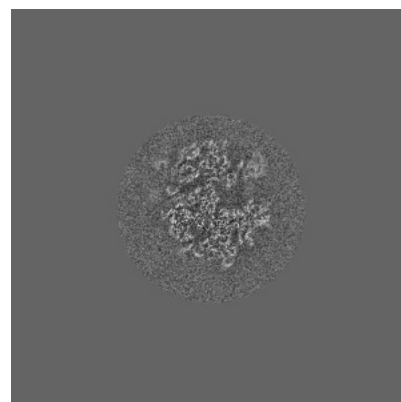
6.2.2 Raw map



X Index: 384



Y Index: 384

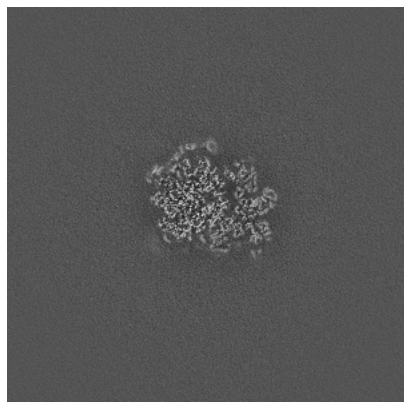


Z Index: 384

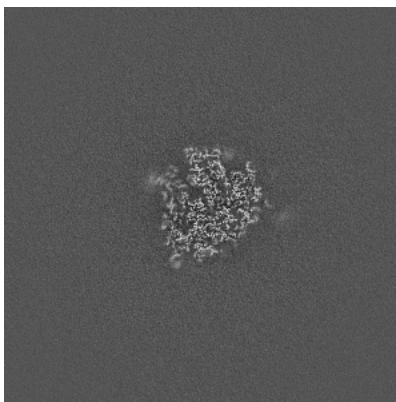
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

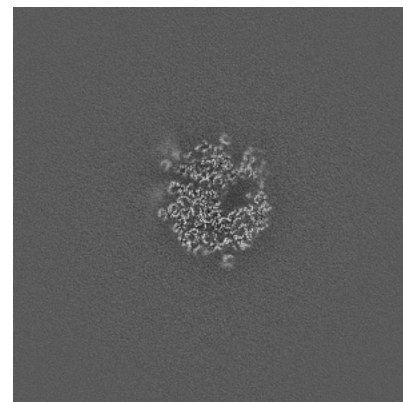
6.3.1 Primary map



X Index: 390

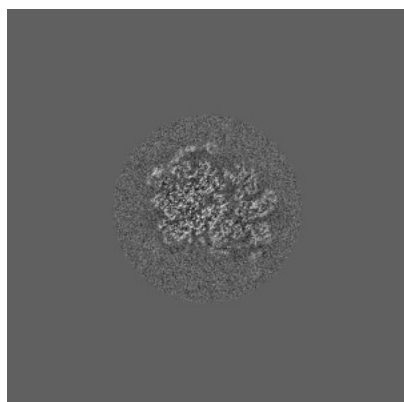


Y Index: 376

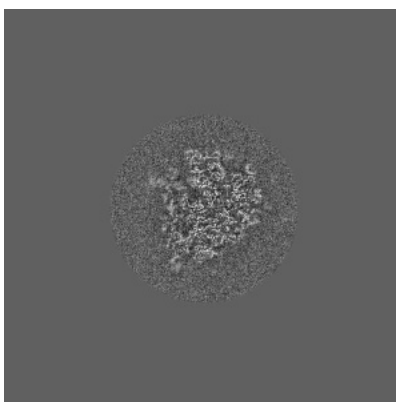


Z Index: 375

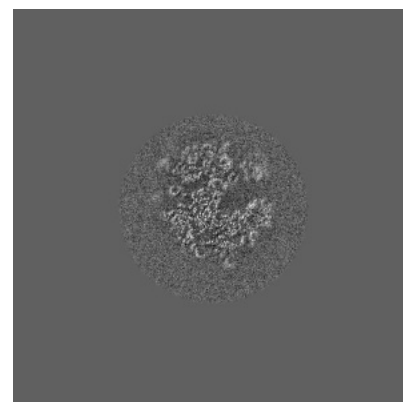
6.3.2 Raw map



X Index: 390



Y Index: 376



Z Index: 381

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



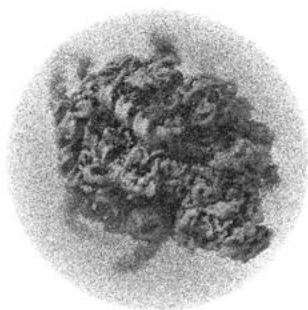
Y



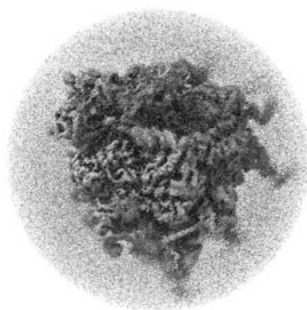
Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

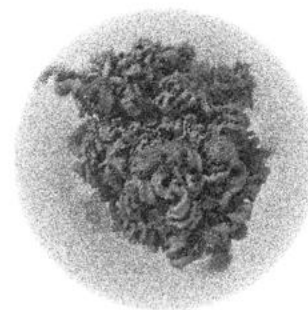
6.4.2 Raw map



X



Y



Z

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

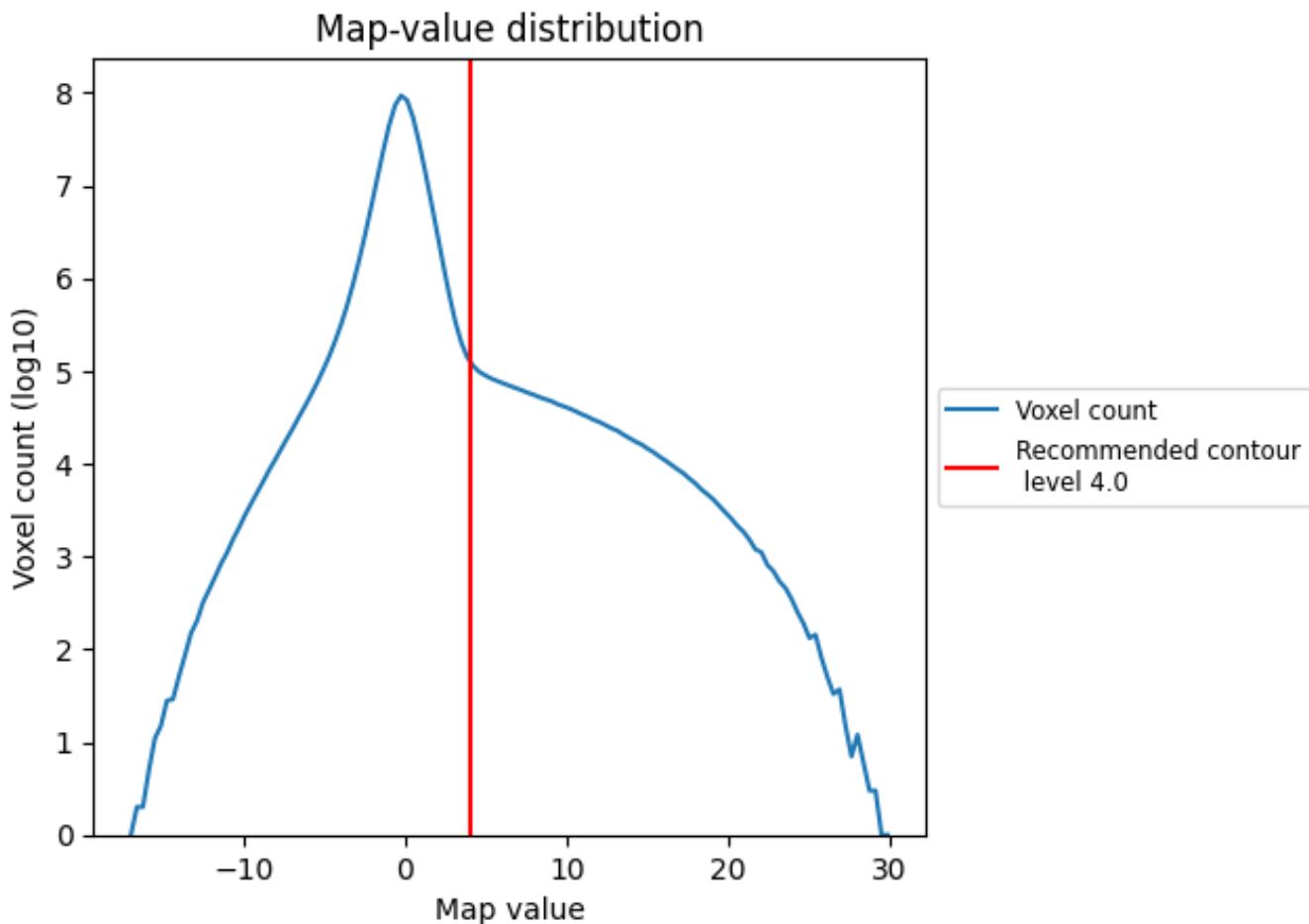
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

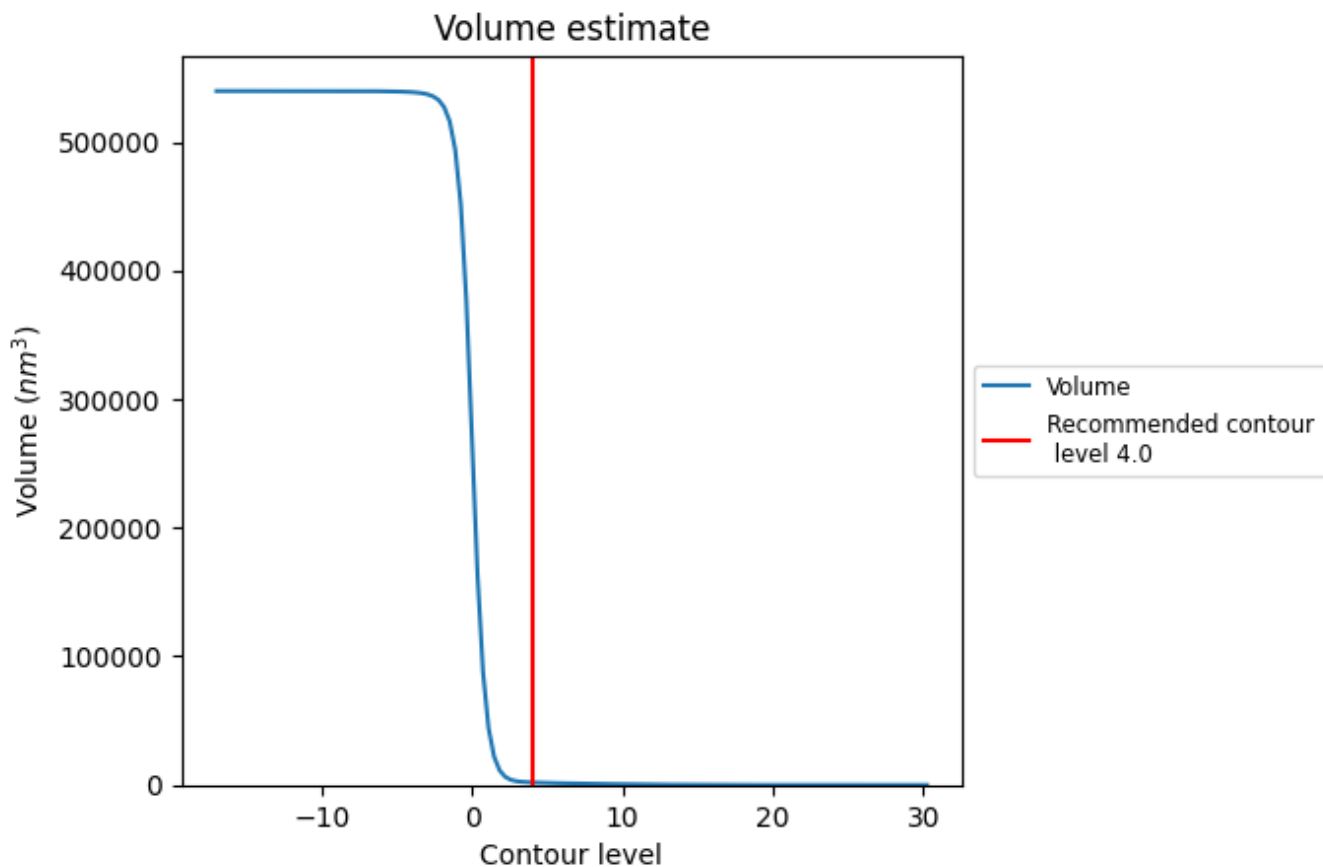
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

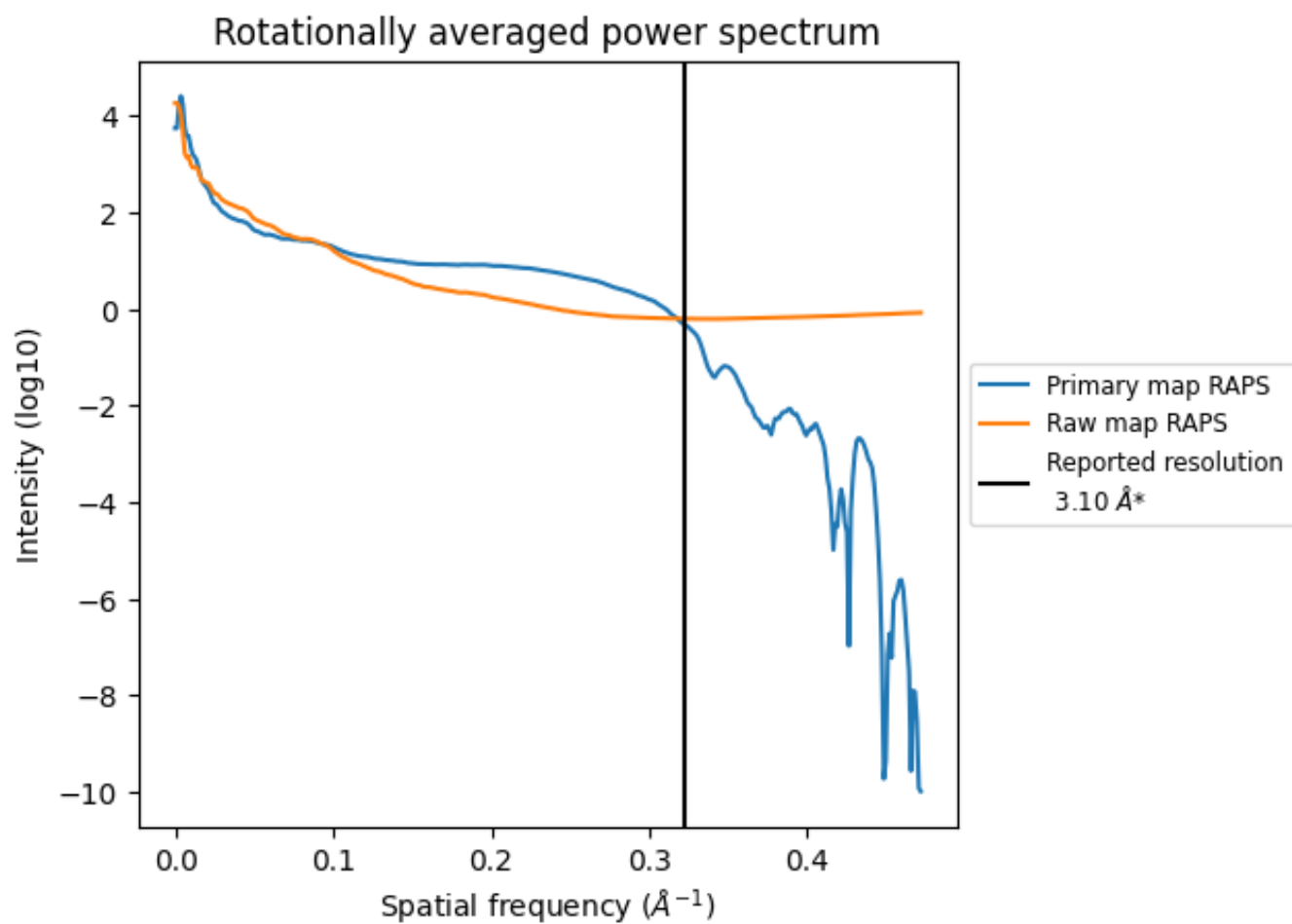
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1947 nm^3 ; this corresponds to an approximate mass of 1759 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

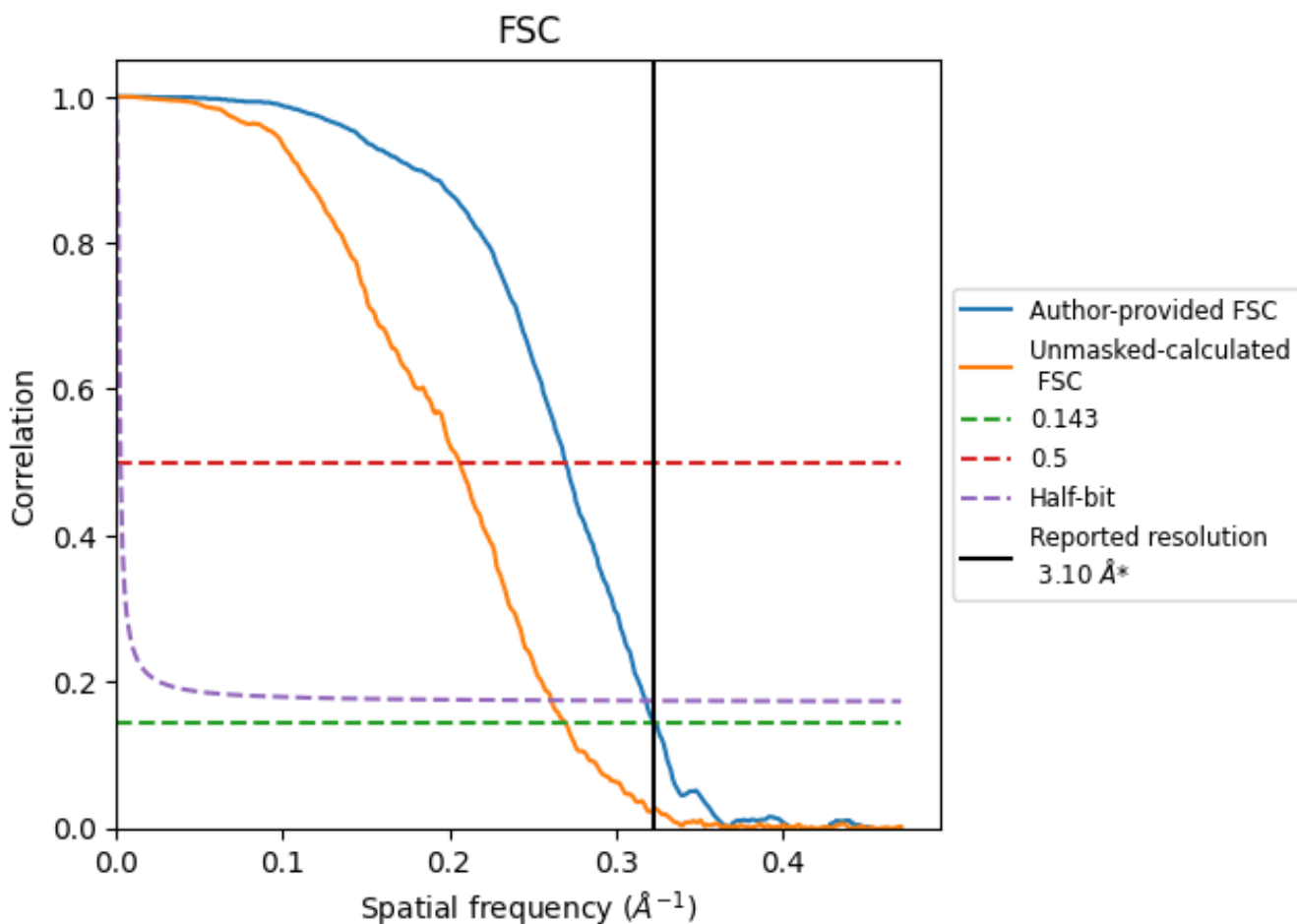


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

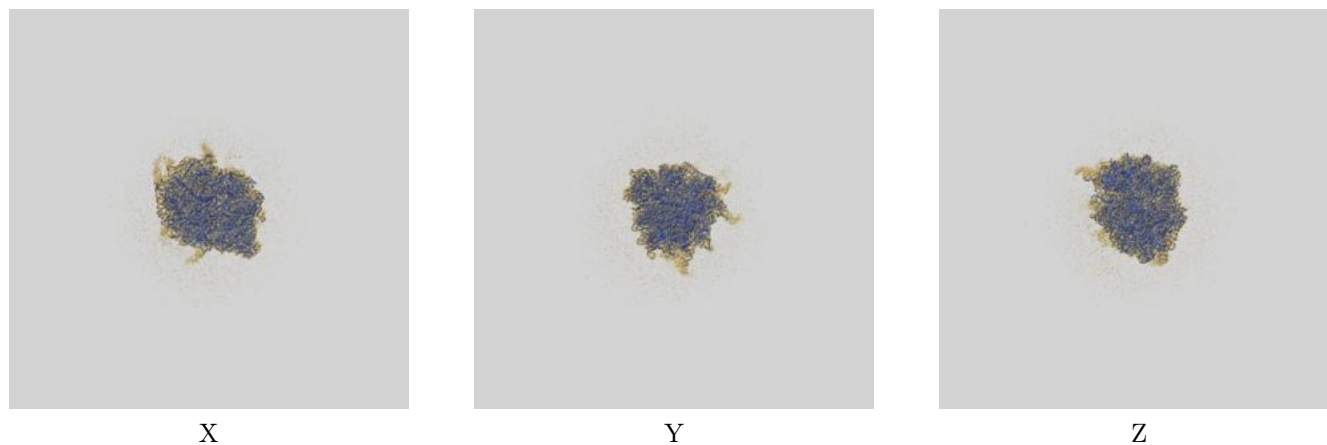
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.71	3.14
Unmasked-calculated*	3.70	4.85	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23501 and PDB model 7LS2. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)

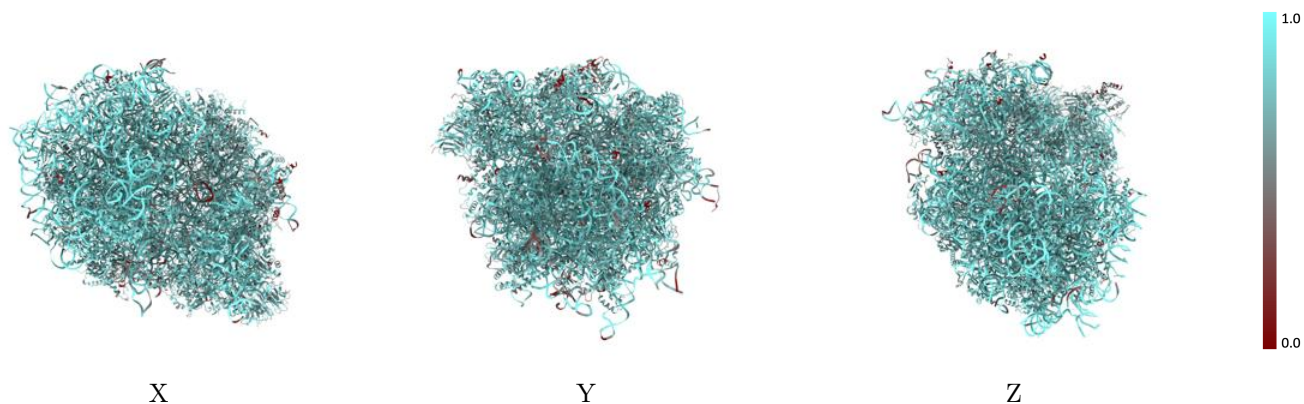


The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

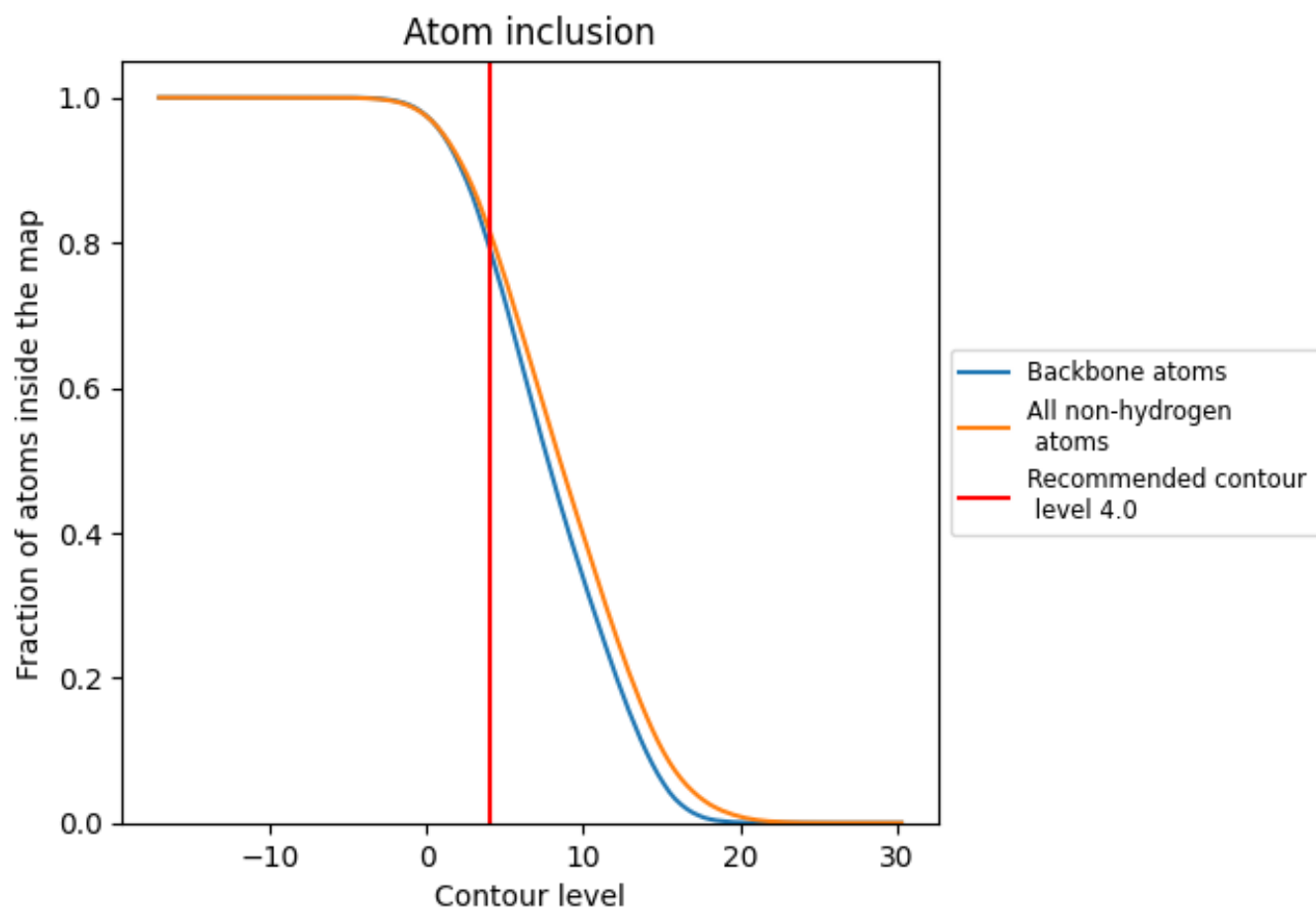
This section was not generated.

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 (4.0).




































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 82% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.8184
A	 0.4705
A1	 0.7782
A2	 0.8968
A3	 0.7118
B1	 0.7881
B2	 0.9543
B3	 0.7435
C1	 0.7799
C2	 0.9041
C3	 0.7137
D1	 0.7735
D2	 0.7594
D3	 0.7781
E1	 0.7677
E2	 0.7827
E3	 0.6947
F1	 0.8063
F2	 0.7789
F3	 0.7426
G1	 0.8208
G2	 0.8278
G3	 0.5947
H1	 0.8019
H2	 0.8040
H3	 0.7472
I2	 0.7933
I3	 0.7378
J2	 0.8093
J3	 0.7493
K2	 0.7849
K3	 0.6940
L1	 0.5417
L2	 0.7776
L3	 0.7304












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Chain	Atom inclusion
M2	 0.8197
M3	 0.5301
N2	 0.7910
N3	 0.7253
O2	 0.7559
O3	 0.7061
P2	 0.7265
P3	 0.7228
Q2	 0.7206
Q3	 0.6742
R2	 0.7830
R3	 0.6792
S2	 0.8006
S3	 0.7297
T2	 0.8155
T3	 0.6974
U2	 0.8142
U3	 0.6829
V2	 0.7272
W2	 0.7944
X2	 0.7888
Y2	 0.7797
Z2	 0.8147
a2	 0.7791
b2	 0.7756
c2	 0.8063
d2	 0.7875
e2	 0.7230
f2	 0.7612
g2	 0.7890
h2	 0.7033
i2	 0.7772
j	 0.7266
j2	 0.7556
k	 0.6280
k2	 0.8347
m	 0.7038
m2	 0.8857
n2	 0.8429
o2	 0.7725
p2	 0.7020
q2	 0.7122

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Chain	Atom inclusion
r2	 0.7156
s2	 0.6481
t	 0.7166
u	 0.6785
v2	 0.7152
w2	 0.6799
x2	 0.7064
y2	 0.7118
z2	 0.7152