Full wwPDB EM Validation Report ⓘ

Dec 17, 2023 – 03:47 AM JST

PDB ID	:	8JDJ
EMDB ID	:	EMD-36178
Title	:	Structure of the Human cytoplasmic Ribosome with human tRNA Asp(Q34) and mRNA(GAU)
Authors	:	Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.
Deposited on	:	2023-05-14
Resolution	:	2.50 Å(reported)
Based on initial model	:	6Y0G

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:

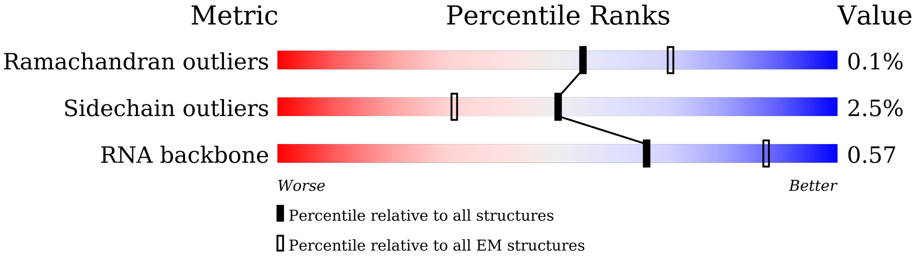
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

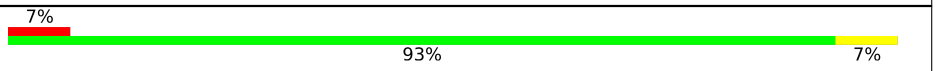
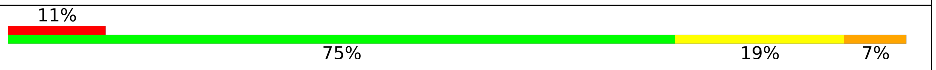
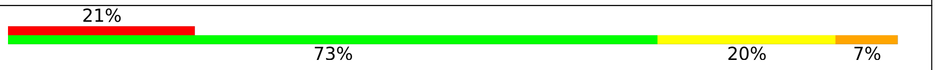
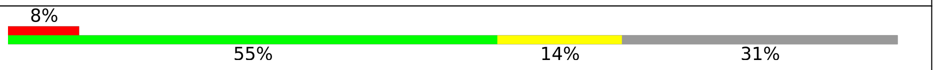
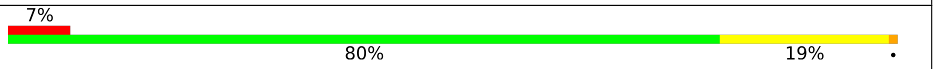
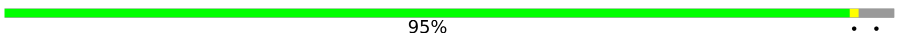
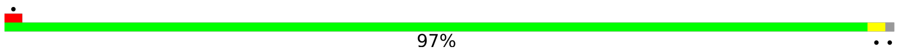
The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	14	
2	B	75	
2	C	75	
3	D	5070	
4	E	120	
5	F	156	
6	G	257	
7	H	403	

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Mol	Chain	Length	Quality of chain
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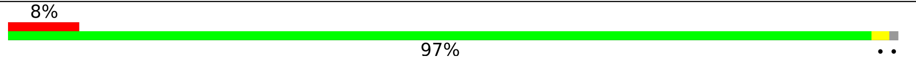
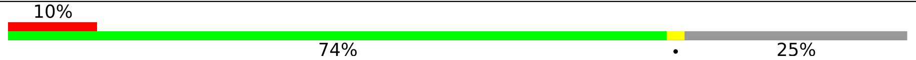
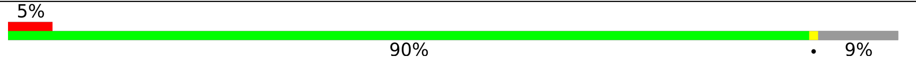
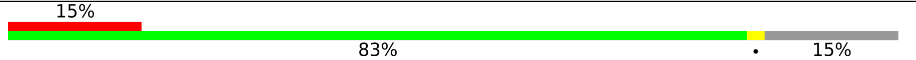
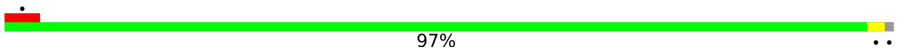
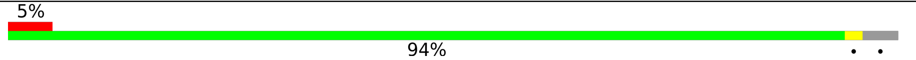
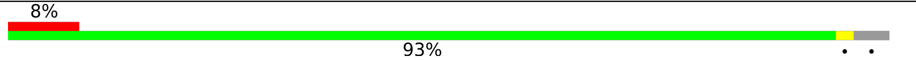
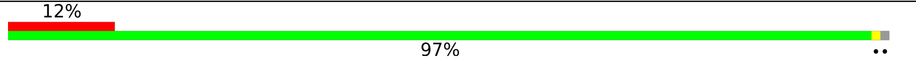
9	J	297	
10	K	288	
11	L	248	
12	M	266	
13	N	192	
14	O	214	
15	P	178	
16	Q	211	
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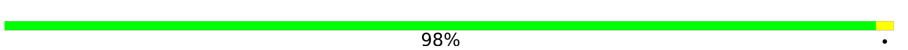
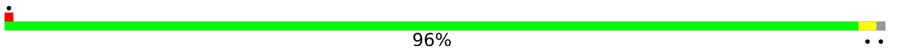
18	S	204	
19	T	203	
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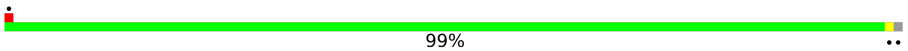
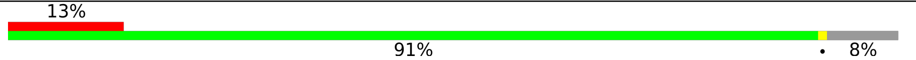
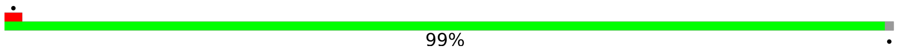
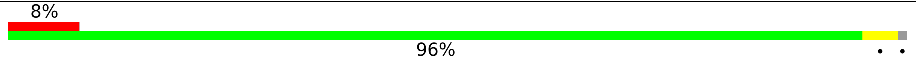
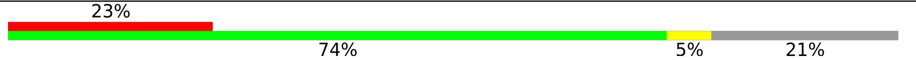
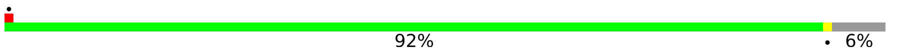
21	V	188	
22	W	196	
23	X	176	
24	Y	160	
25	Z	128	
26	a	140	
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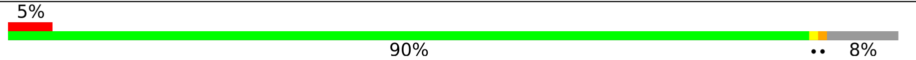
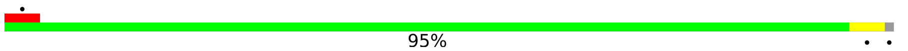
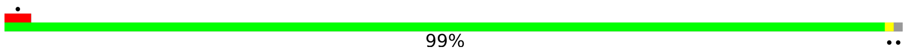
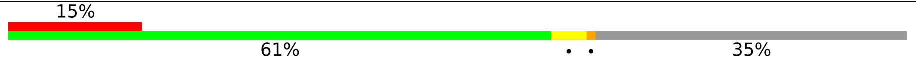
28	c	156	
29	d	145	
30	e	136	
31	f	148	
32	g	159	

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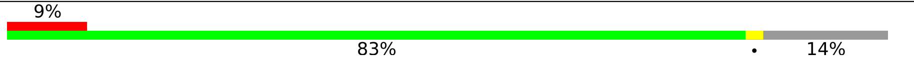
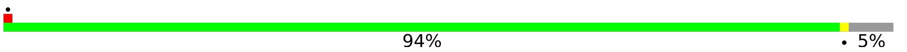
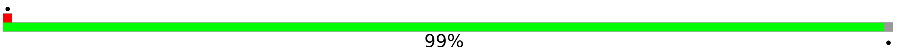
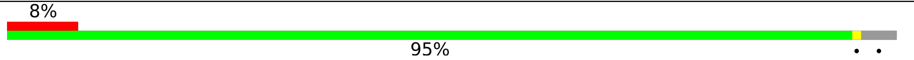
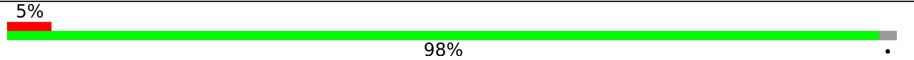
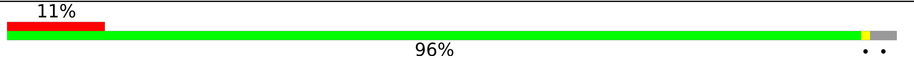
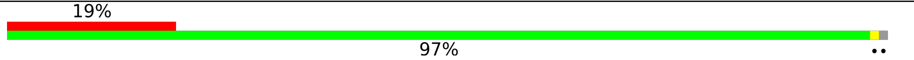
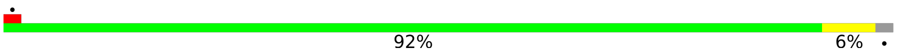
Mol	Chain	Length	Quality of chain
33	h	115	
34	i	125	
35	j	135	
36	k	110	
37	l	117	
38	m	123	
39	n	105	
40	o	97	
41	p	70	
42	q	51	
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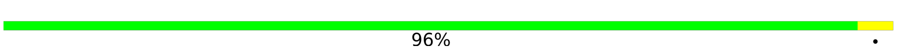
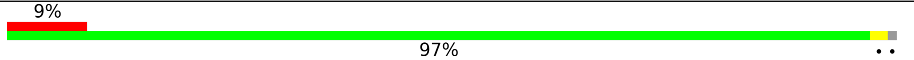
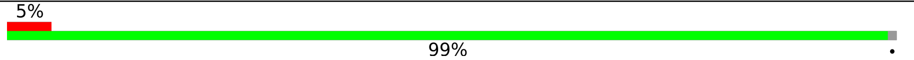
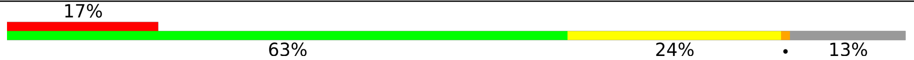
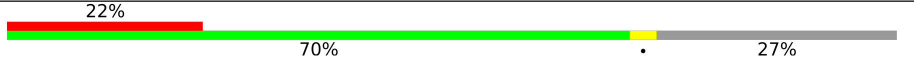
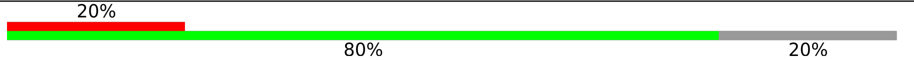
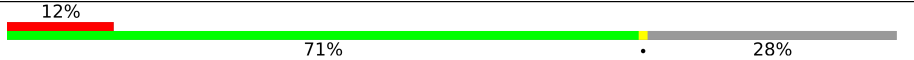
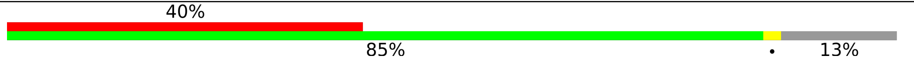
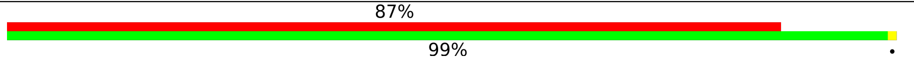
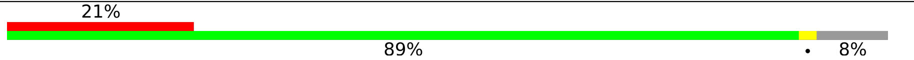
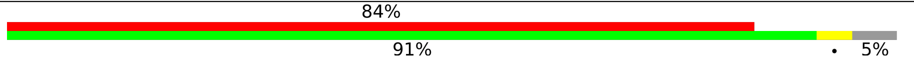
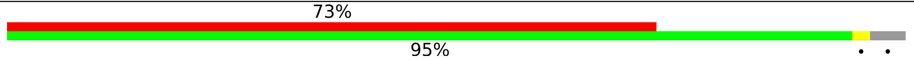
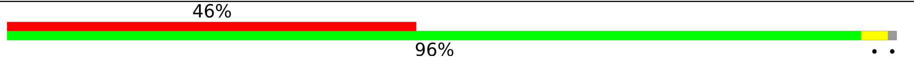
44	s	25	
45	t	106	
46	u	92	
47	v	137	
48	w	1869	
49	x	295	
50	y	264	
51	z	293	
52	0	243	
53	1	263	
54	2	204	
55	3	249	
56	4	194	
57	5	208	

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Mol	Chain	Length	Quality of chain
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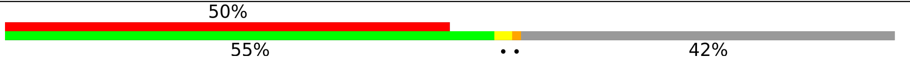
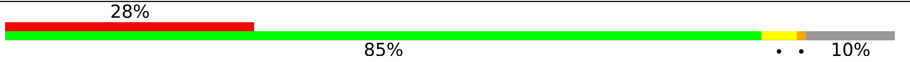
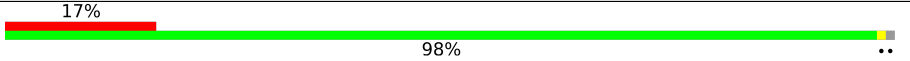
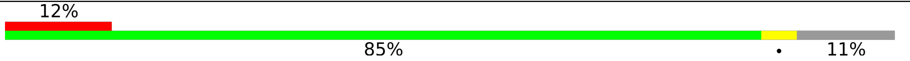
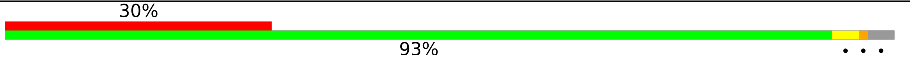
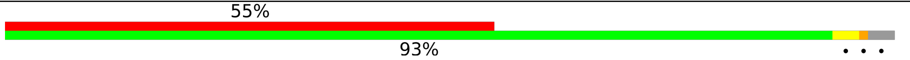
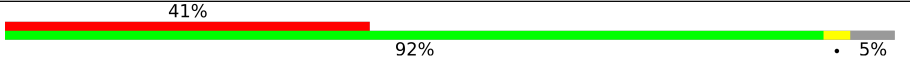
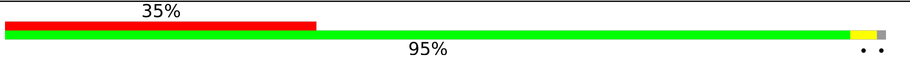
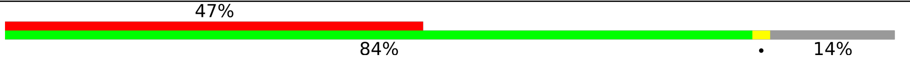
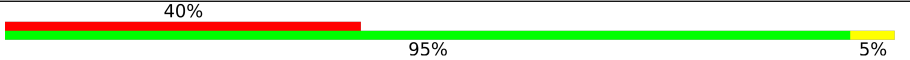
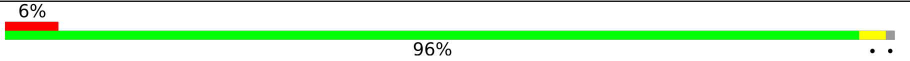
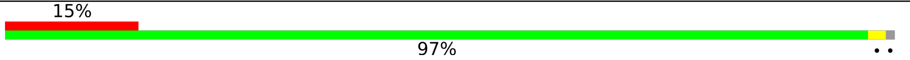
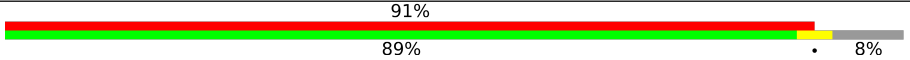
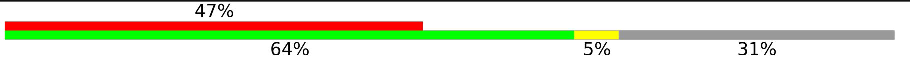
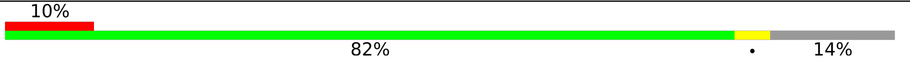
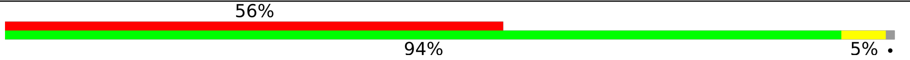
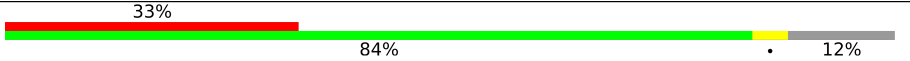
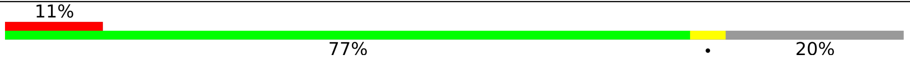
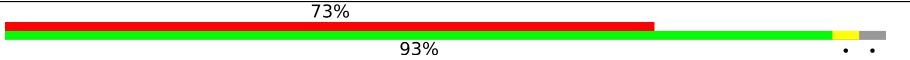
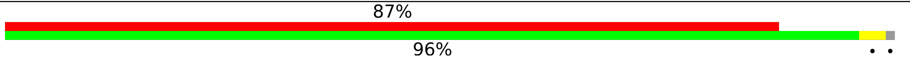
59	7	165	
60	8	158	
61	9	151	
62	AA	151	
63	AB	145	
64	AC	146	
65	AD	135	
66	AE	152	
67	AF	145	
68	AG	119	
69	AH	83	
70	AI	130	
71	AJ	143	
72	AK	133	
73	AL	125	
74	AM	115	
75	AN	84	
76	AO	69	
77	AP	56	
78	AQ	59	
79	AR	317	

2 Entry composition ⓘ

There are 81 unique types of molecules in this entry. The entry contains 209545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	14	303	135	55	99	14	0	0

- Molecule 2 is a RNA chain called tRNA(Asp).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	75	1612	726	283	529	74	0	0
2	C	75	1612	726	283	529	74	0	0

- Molecule 3 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	D	3512	75336	33585	13757	24482	3512	0	0

- Molecule 4 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 5 is a RNA chain called 5.8S ribosomal RNA.

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

- Molecule 6 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	247	1891	1185	388	312	6	0	0

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	398	3211	2045	604	548	14	0	0

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	363	2884	1815	577	478	14	0	0

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	293	2379	1506	434	425	14	0	0

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	217	1751	1128	332	287	4	0	0

- Molecule 11 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	225	1870	1202	358	301	9	0	0

- Molecule 12 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	227	1832	1168	352	308	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	190	1518	956	284	272	6	0	0

- Molecule 14 is a protein called 60S ribosomal protein L10-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	206	1660	1053	319	275	13	0	0

- Molecule 15 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	170	1362	861	254	241	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	208	1682	1052	348	278	4	0	0

- Molecule 17 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	136	1120	719	215	179	7	0	0

- Molecule 18 is a protein called 60S ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	200	1641	1058	320	258	5	0	0

- Molecule 20 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	157	Total 1273	C 797	N 246	O 221	S 9	0	0

- Molecule 21 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	187	Total 1513	C 944	N 314	O 250	S 5	0	0

- Molecule 22 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	180	Total 1508	C 933	N 328	O 238	S 9	0	0

- Molecule 23 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	175	Total 1453	C 925	N 283	O 235	S 10	0	0

- Molecule 24 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	159	Total 1298	C 823	N 252	O 217	S 6	0	0

- Molecule 25 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	101	Total 821	C 526	N 143	O 150	S 2	0	0

- Molecule 26 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	131	Total 979	C 618	N 184	O 172	S 5	0	0

- Molecule 27 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	63	528	337	103	85	3	0	0

- Molecule 28 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	120	981	628	185	167	1	0	0

- Molecule 29 is a protein called 60S ribosomal protein L26.

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

- Molecule 30 is a protein called 60S ribosomal protein L27.

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

- Molecule 31 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	147	1162	736	237	186	3	0	0

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	104	832	515	182	132	3	0	0

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	97	755	479	133	137	6	0	0

- Molecule 34 is a protein called 60S ribosomal protein L31.

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

- Molecule 35 is a protein called 60S ribosomal protein L32.

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

- Molecule 36 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 37 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	112	Total	C	N	O	S	0	0
			888	555	183	144	6		

- Molecule 38 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	121	Total	C	N	O	S	0	0
			1010	638	204	167	1		

- Molecule 39 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 40 is a protein called 60S ribosomal protein L37.

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

- Molecule 41 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	69	569	366	103	99	1	0	0

- Molecule 42 is a protein called 60S ribosomal protein L39.

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

- Molecule 43 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	52	429	266	90	67	6	0	0

- Molecule 44 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	s	25	239	145	64	27	3	0	0

- Molecule 45 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	t	105	862	542	175	139	6	0	0

- Molecule 46 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	u	91	708	445	136	120	7	0	0

- Molecule 47 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	v	125	1002	622	207	168	5	0	0

- Molecule 48 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	1634	Total 34933	C 15622	N 6267	O 11411	P 1633	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	215	Total 1695	C 1077	N 297	O 313	S 8	0	0

- Molecule 50 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	212	Total 1725	C 1096	N 308	O 307	S 14	0	0

- Molecule 51 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	212	Total 1633	C 1059	N 279	O 285	S 10	0	0

- Molecule 52 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	212	Total 1646	C 1050	N 299	O 290	S 7	0	0

- Molecule 53 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	262	Total 2070	C 1321	N 383	O 358	S 8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	187	Total 1464	C 916	N 276	O 265	S 7	0	0

- Molecule 55 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	3	237	1917	1197	384	329	7	0	0

- Molecule 56 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	4	187	1510	963	278	268	1	0	0

- Molecule 57 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	5	206	1674	1049	329	291	5	0	0

- Molecule 58 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	6	182	1506	959	300	245	2	0	0

- Molecule 59 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	7	96	810	530	143	131	6	0	0

- Molecule 60 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	8	142	1150	732	215	197	6	0	0

- Molecule 61 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	9	150	1208	773	229	205	1	0	0

- Molecule 62 is a protein called 40S ribosomal protein S14.

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

- Molecule 63 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	AB	134	1103	703	208	185	7	0	0

- Molecule 64 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	AC	142	1128	717	213	195	3	0	0

- Molecule 65 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	AD	131	1057	665	197	191	4	0	0

- Molecule 66 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	AE	144	1169	731	236	201	1	0	0

- Molecule 67 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	AF	143	1111	696	213	198	4	0	0

- Molecule 68 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	AG	102	799	501	153	141	4	0	0

- Molecule 69 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AH	83	Total 636	C 393	N 117	O 121	S 5	0	0

- Molecule 70 is a protein called 40S ribosomal protein S15a.

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

- Molecule 71 is a protein called 40S ribosomal protein S23.

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

- Molecule 72 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AK	123	Total 1002	C 634	N 196	O 167	S 5	0	0

- Molecule 73 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AL	86	Total 680	C 436	N 127	O 116	S 1	0	0

- Molecule 74 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AM	99	Total 792	C 492	N 165	O 130	S 5	0	0

- Molecule 75 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AN	83	Total 643	C 402	N 119	O 115	S 7	0	0

- Molecule 76 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	AO	61	479	292	95	90	2	0	0

- Molecule 77 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	AP	45	370	228	77	60	5	0	0

- Molecule 78 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	AQ	57	452	279	99	73	1	0	0

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 80 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
80	A	1	1	1	0
80	D	398	398	398	0
80	E	10	10	10	0
80	F	6	6	6	0
80	G	2	2	2	0
80	H	1	1	1	0
80	I	1	1	1	0
80	N	1	1	1	0
80	O	2	2	2	0

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Mol	Chain	Residues	Atoms		AltConf
80	S	1	Total 1	Mg 1	0
80	U	2	Total 2	Mg 2	0
80	V	2	Total 2	Mg 2	0
80	X	1	Total 1	Mg 1	0
80	a	1	Total 1	Mg 1	0
80	g	1	Total 1	Mg 1	0
80	j	1	Total 1	Mg 1	0
80	k	1	Total 1	Mg 1	0
80	l	1	Total 1	Mg 1	0
80	u	1	Total 1	Mg 1	0
80	w	103	Total 103	Mg 103	0
80	AA	1	Total 1	Mg 1	0
80	AF	1	Total 1	Mg 1	0

- Molecule 81 is ZINC ION (three-letter code: ZN) (formula: Zn).

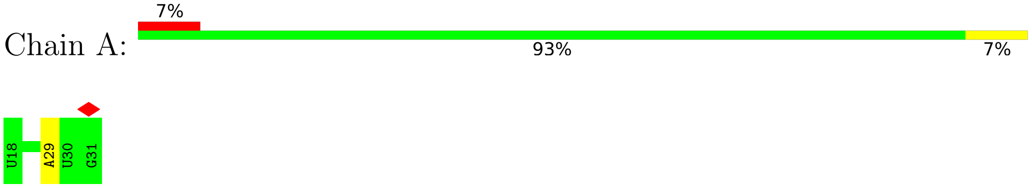
Mol	Chain	Residues	Atoms		AltConf
81	o	1	Total 1	Zn 1	0
81	r	1	Total 1	Zn 1	0
81	t	1	Total 1	Zn 1	0
81	u	1	Total 1	Zn 1	0
81	AM	1	Total 1	Zn 1	0
81	AP	1	Total 1	Zn 1	0

3 Residue-property plots ⓘ

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

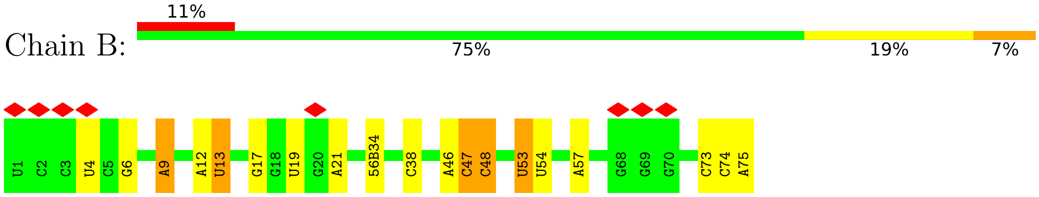
- Molecule 1: mRNA

Chain A:



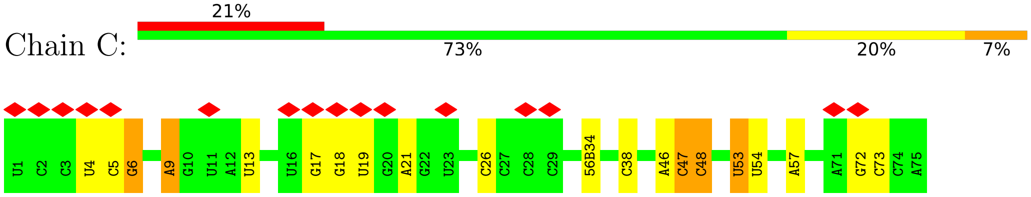
- Molecule 2: tRNA(Asp)

Chain B:



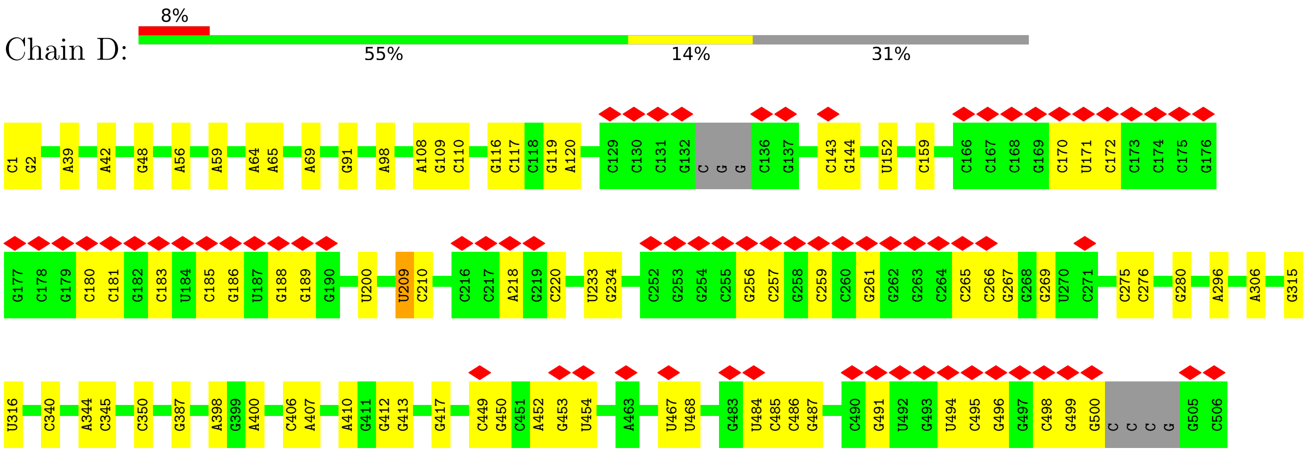
- Molecule 2: tRNA(Asp)

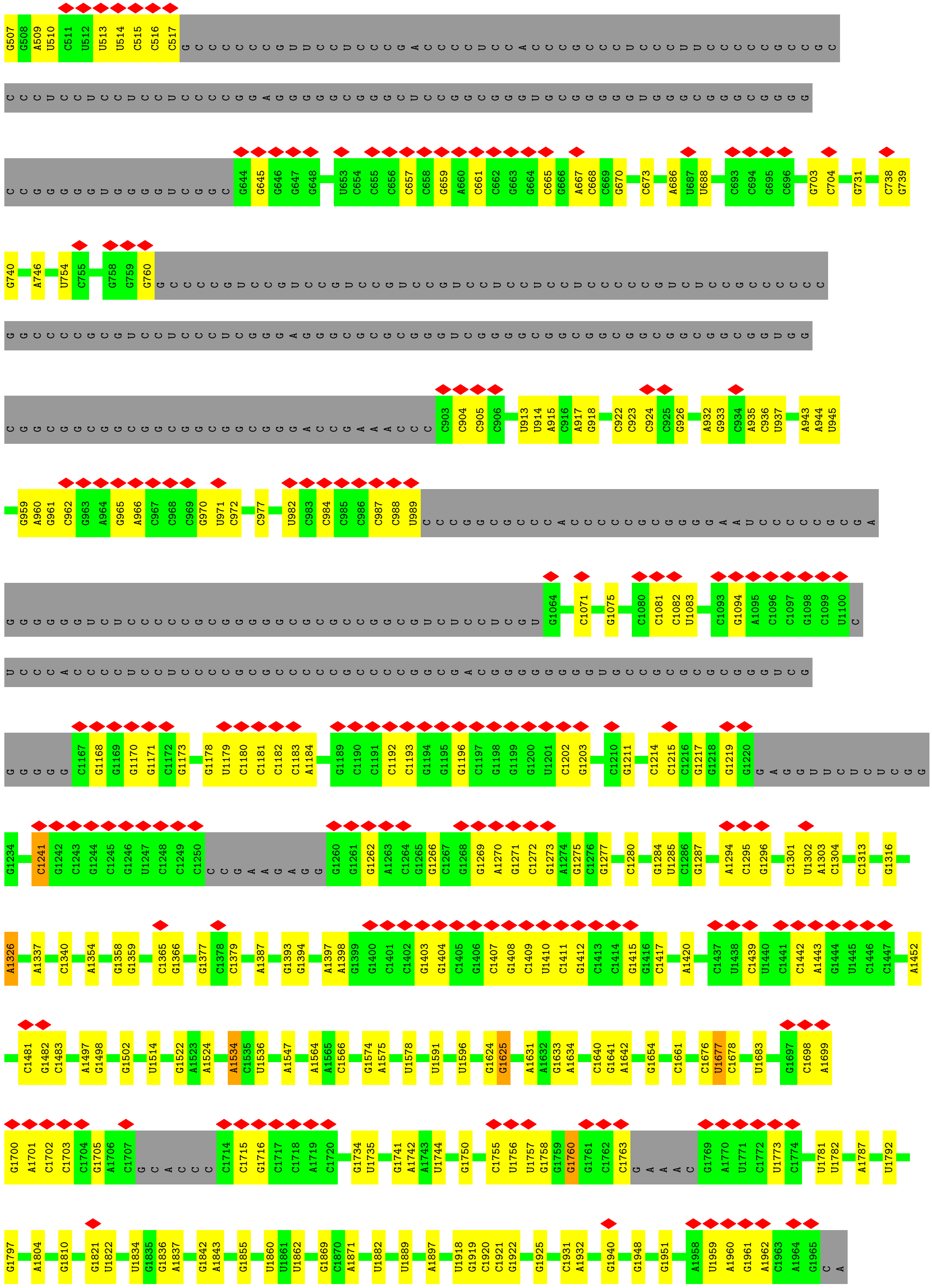
Chain C:



- Molecule 3: 28S ribosomal RNA

Chain D:




G507 G508 A509 U510 C511 U512 U513 U514 C515 C516 C517 G C C C C C C G U U C C U C C C G A C C C C U C C A C C C G C C C U C C C U U C C C C C G C C G C
C C C U C C U C C U C C U C C C C G G A G G G G G C G G G C U C C G G C G G G U G C G G G G G U G G G C G G G C G G G G
C C G G G G G U G G G G U C G G C G644 G645 G646 G647 G648 U653 C654 C655 C656 C657 C658 G659 A660 C661 C662 G663 G664 C665 G666 A667 C668 C669 G670 C673 A686 U687 U688 C693 C694 G695 C696 G703 C704 G731 C738 G739
G740 A746 U754 C755 G758 G759 G760 G C C C C G U C C G U C C G U C C G U C C G U C C U C C U C C U C C C C C G U C U C C G C C C C C C
G G C C C C G C G U C C U C C C U C G G G A G G G C G C G C G G G U C G G G G C G G C G G C G G C G G C G G U G G
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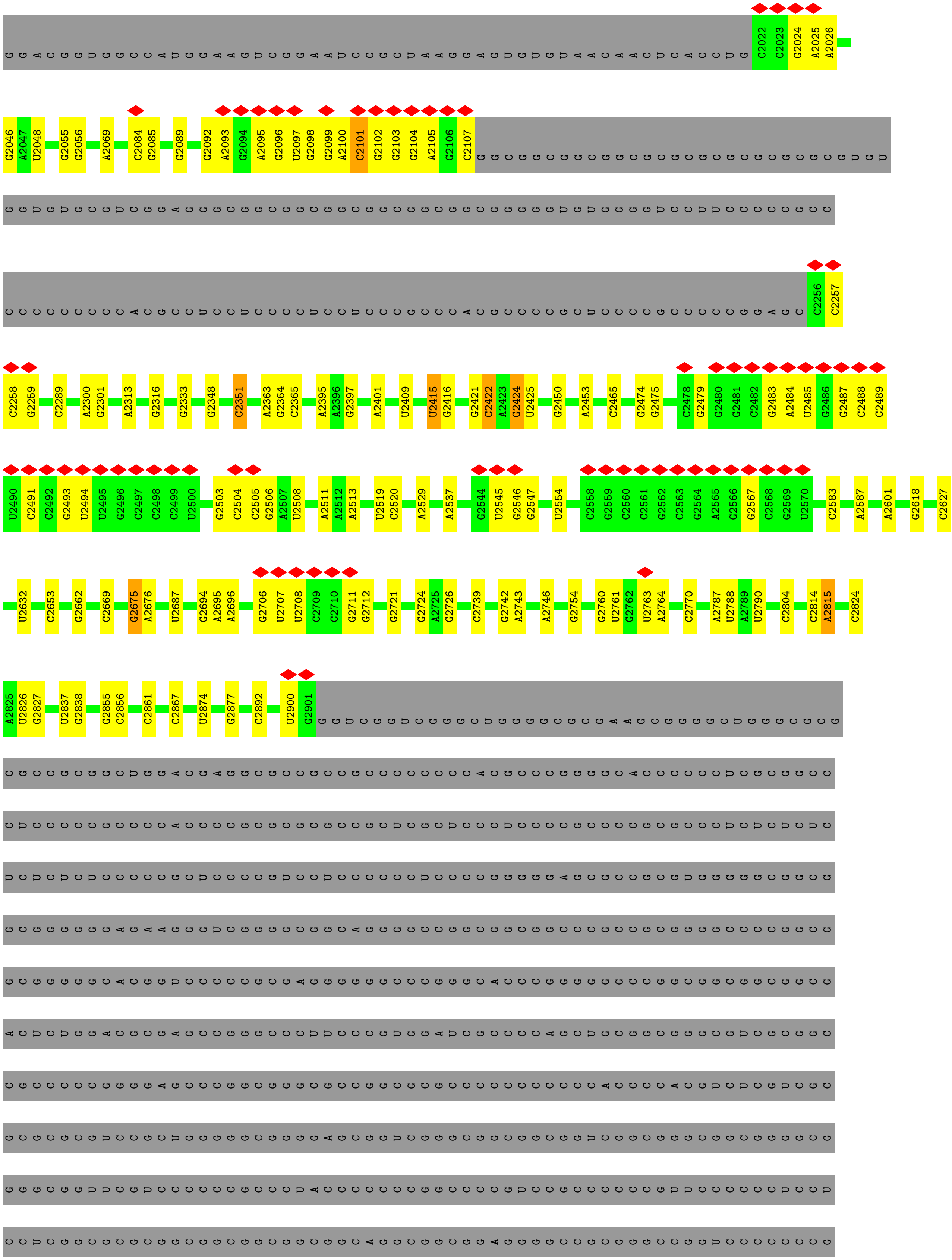
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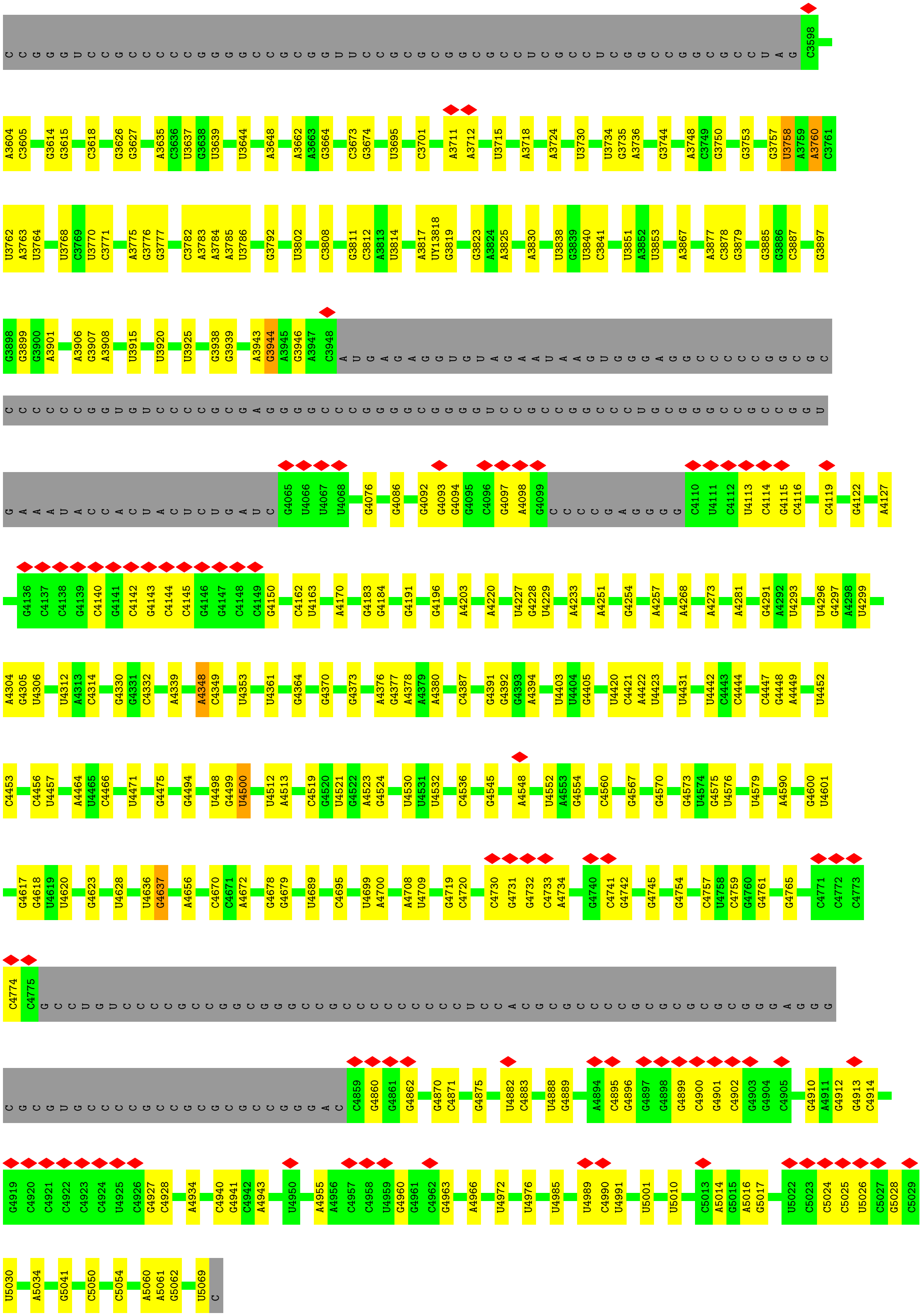
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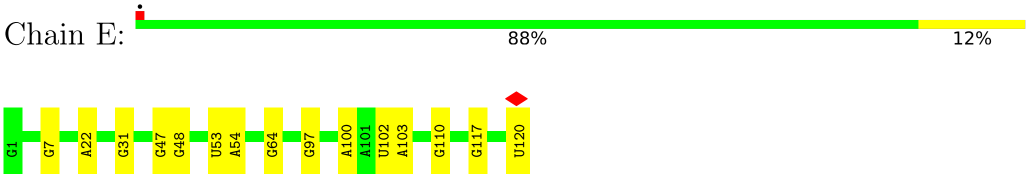
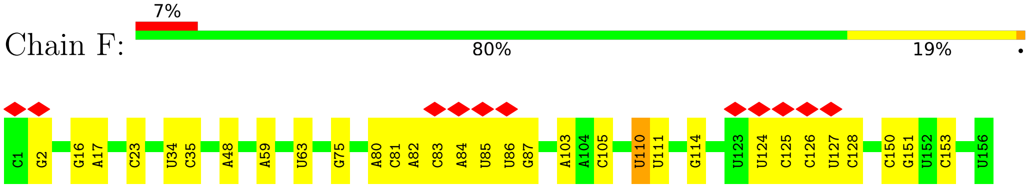
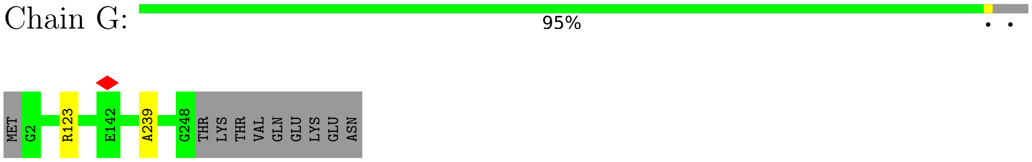
- Molecule 4: 5S ribosomal RNA



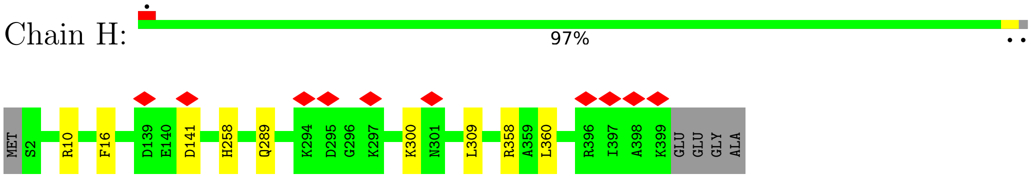
- Molecule 5: 5.8S ribosomal RNA



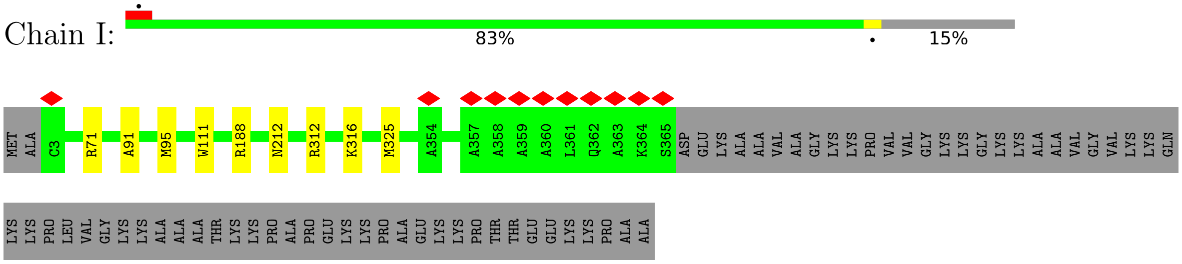
- Molecule 6: 60S ribosomal protein L8



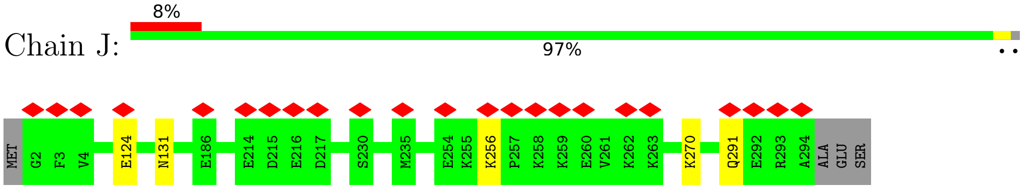
- Molecule 7: 60S ribosomal protein L3



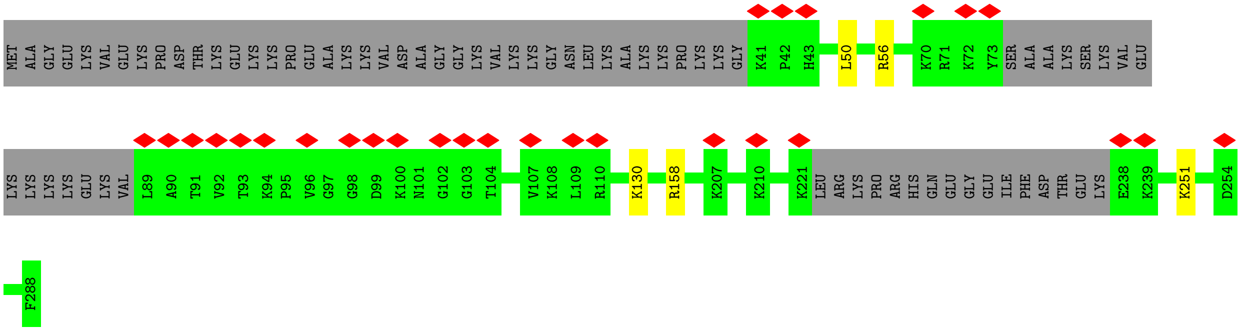
- Molecule 8: 60S ribosomal protein L4



- Molecule 9: 60S ribosomal protein L5



- Molecule 10: 60S ribosomal protein L6



- Molecule 11: 60S ribosomal protein L7

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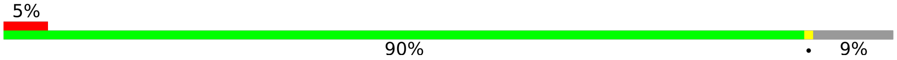
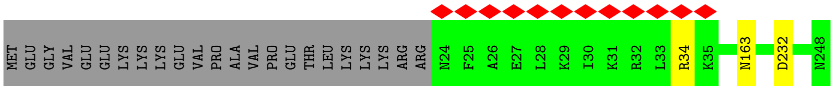
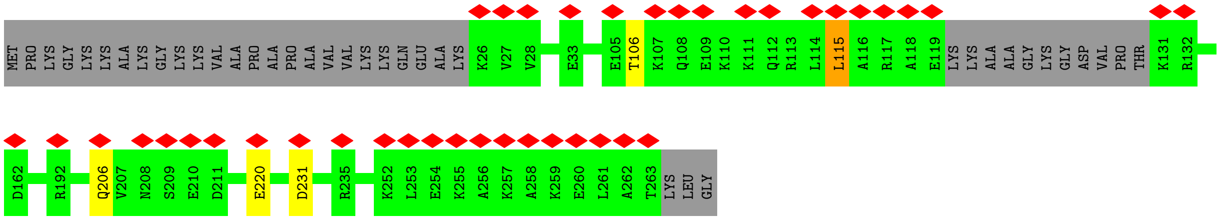




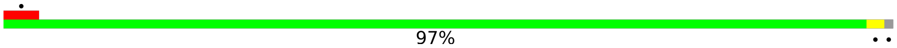
- Molecule 12: 60S ribosomal protein L7a

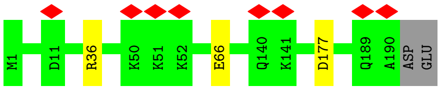
Chain M:



- Molecule 13: 60S ribosomal protein L9

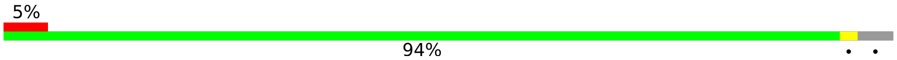
Chain N:

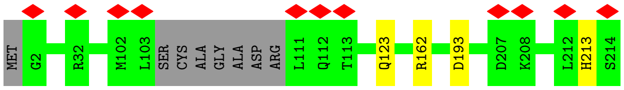




- Molecule 14: 60S ribosomal protein L10-like

Chain O:





- Molecule 15: 60S ribosomal protein L11

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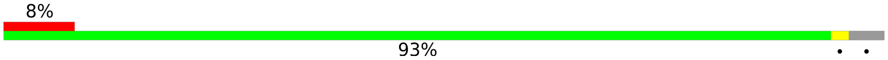

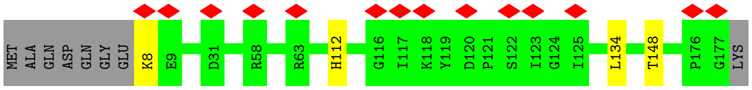

- Molecule 16: 60S ribosomal protein L13

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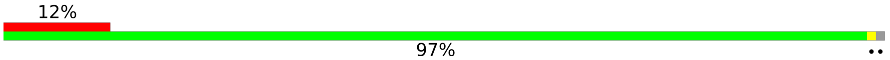
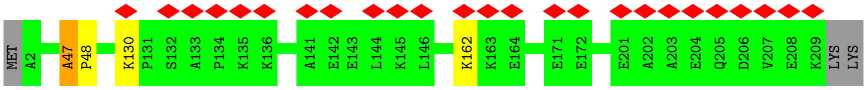
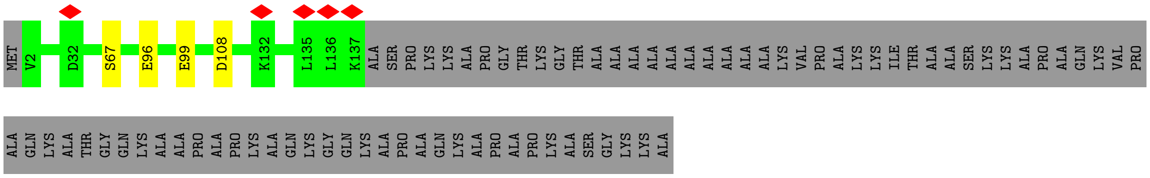




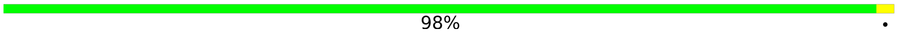
- Molecule 17: 60S ribosomal protein L14

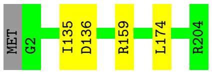
Chain R:



- Molecule 18: 60S ribosomal protein L15

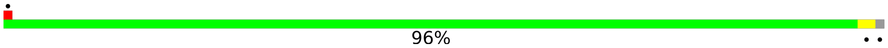
Chain S:

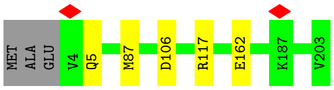




- Molecule 19: 60S ribosomal protein L13a

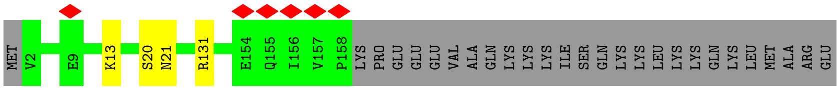
Chain T:





- Molecule 20: 60S ribosomal protein L17

Chain U:



- Molecule 21: 60S ribosomal protein L18

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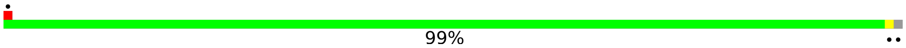
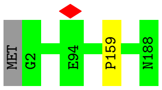
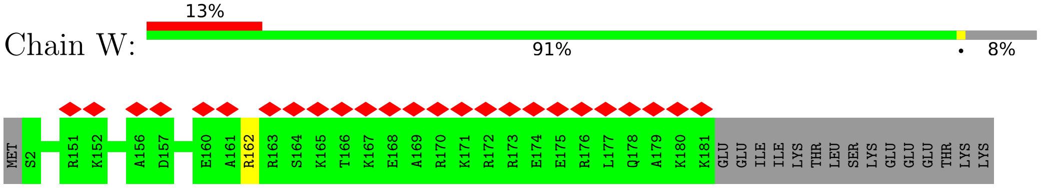




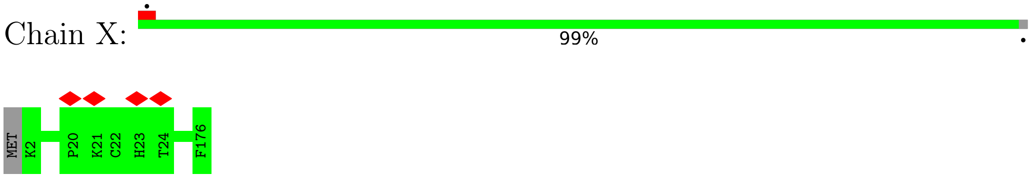
- Molecule 22: 60S ribosomal protein L19

Chain W:



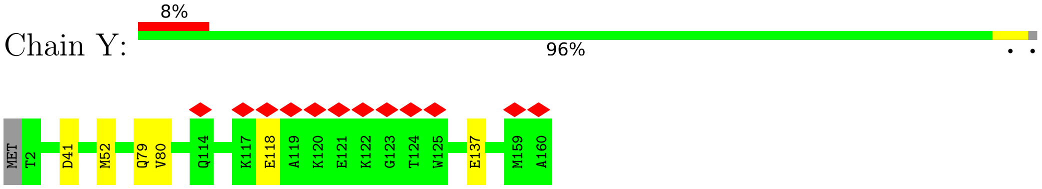
- Molecule 23: 60S ribosomal protein L18a

Chain X:



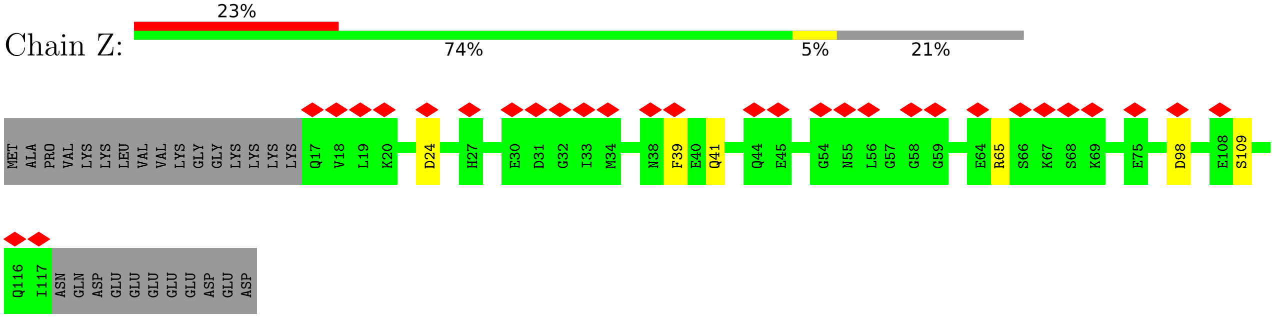
- Molecule 24: 60S ribosomal protein L21

Chain Y:



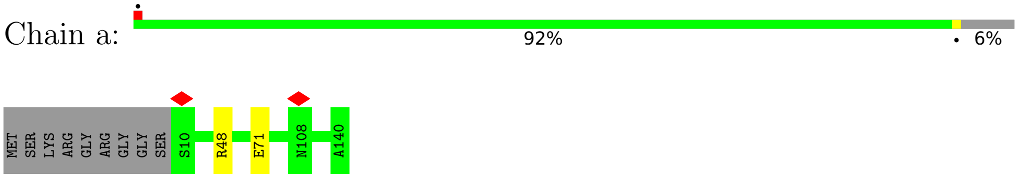
- Molecule 25: 60S ribosomal protein L22

Chain Z:



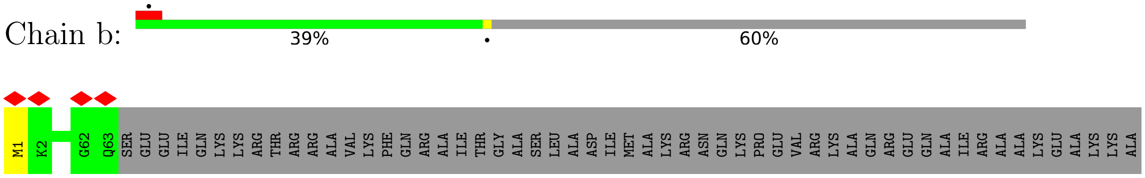
- Molecule 26: 60S ribosomal protein L23

Chain a:

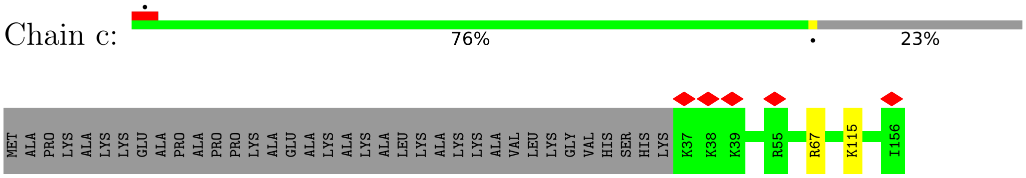


- Molecule 27: 60S ribosomal protein L24

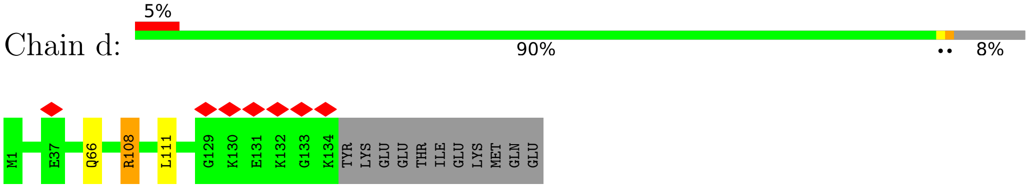
Chain b:



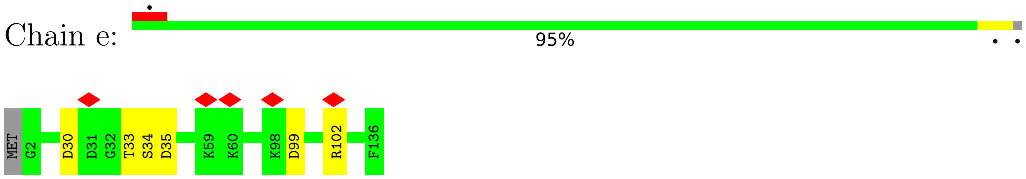
- Molecule 28: 60S ribosomal protein L23a



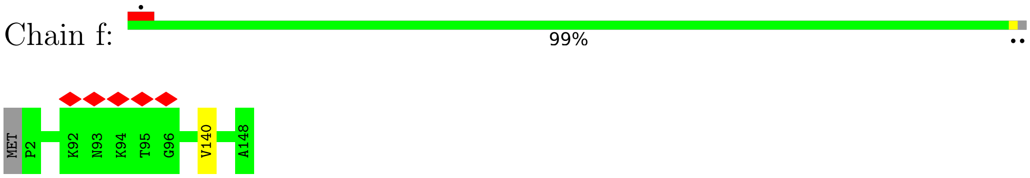
- Molecule 29: 60S ribosomal protein L26



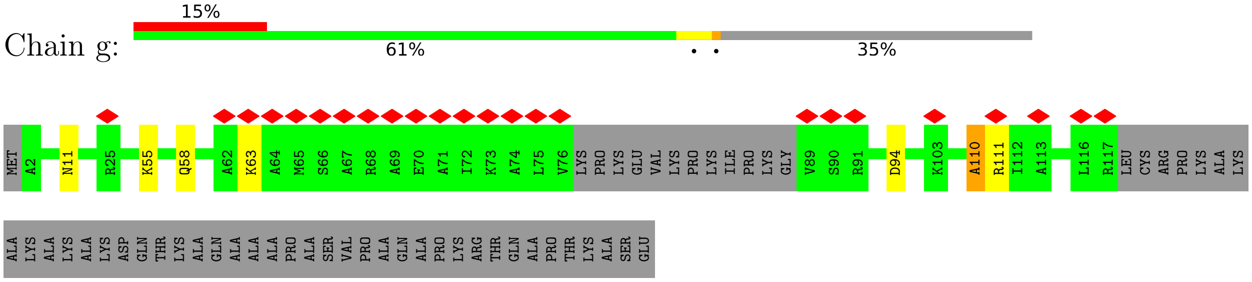
- Molecule 30: 60S ribosomal protein L27



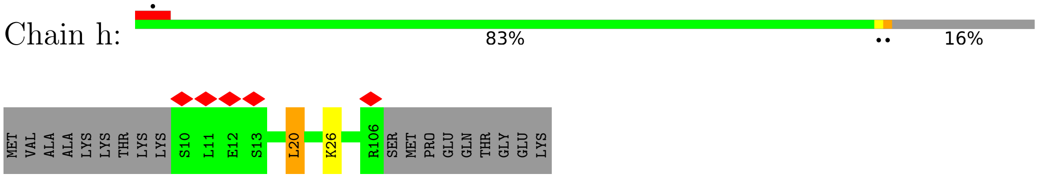
- Molecule 31: 60S ribosomal protein L27a



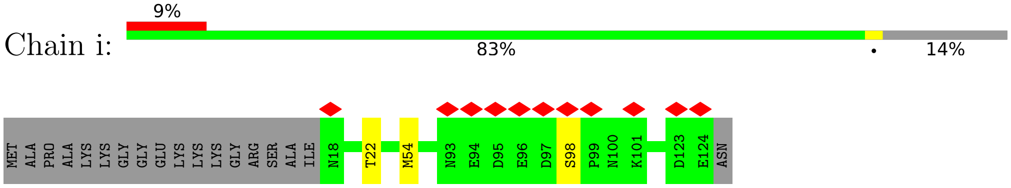
- Molecule 32: 60S ribosomal protein L29



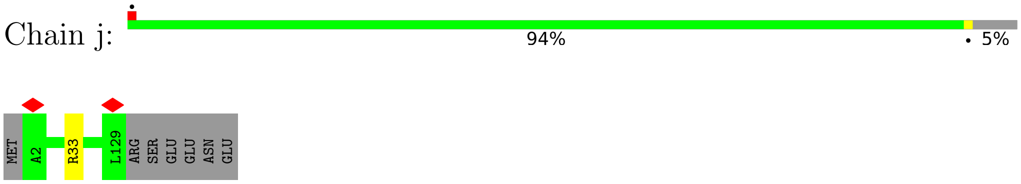
- Molecule 33: 60S ribosomal protein L30



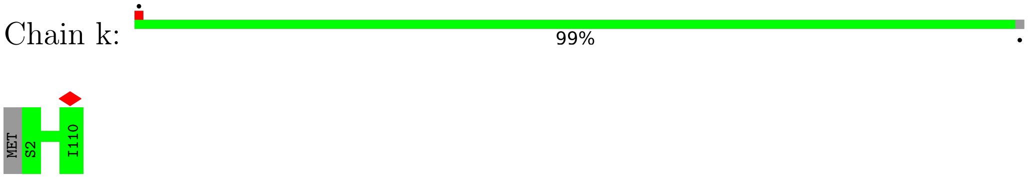
- Molecule 34: 60S ribosomal protein L31



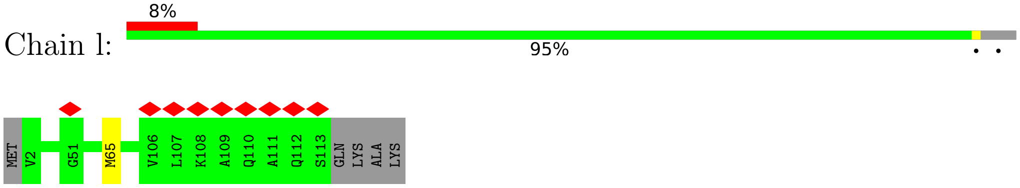
- Molecule 35: 60S ribosomal protein L32



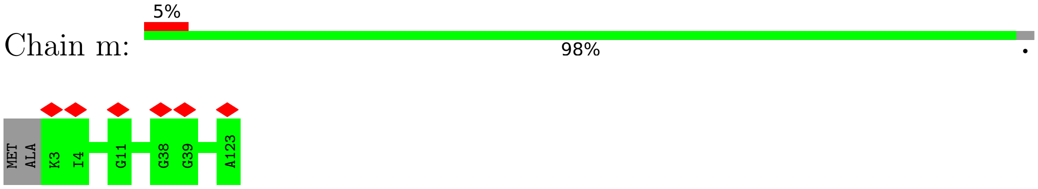
- Molecule 36: 60S ribosomal protein L35a



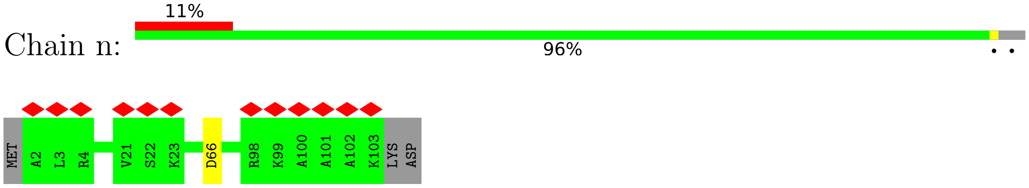
- Molecule 37: 60S ribosomal protein L34



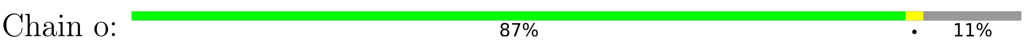
- Molecule 38: 60S ribosomal protein L35

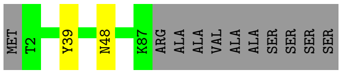


- Molecule 39: 60S ribosomal protein L36



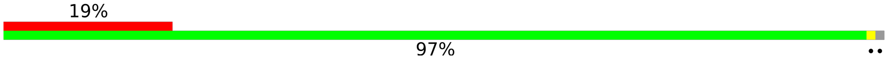
- Molecule 40: 60S ribosomal protein L37

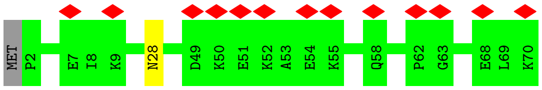




- Molecule 41: 60S ribosomal protein L38

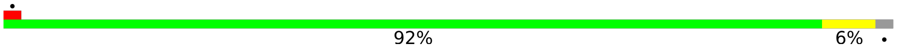
Chain p:

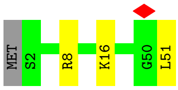




- Molecule 42: 60S ribosomal protein L39

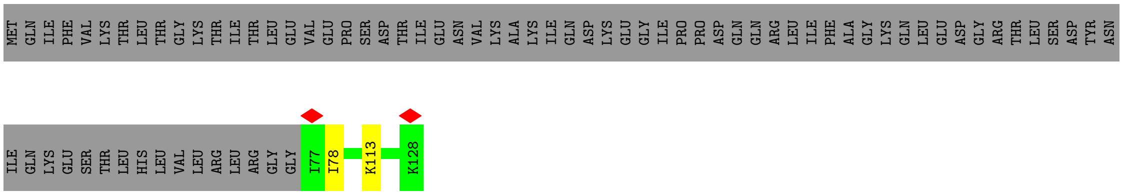
Chain q:





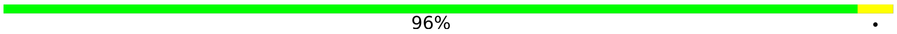
- Molecule 43: Ubiquitin-60S ribosomal protein L40

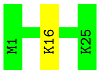
Chain r:



- Molecule 44: 60S ribosomal protein L41

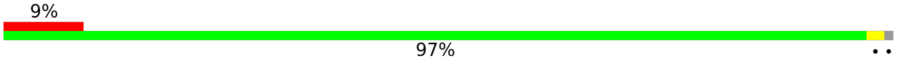
Chain s:

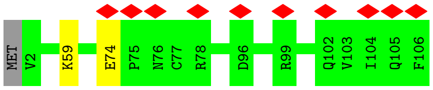




- Molecule 45: 60S ribosomal protein L36a

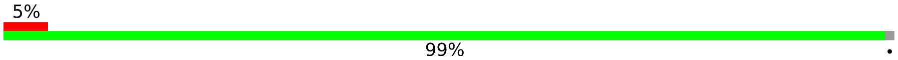
Chain t:

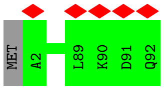




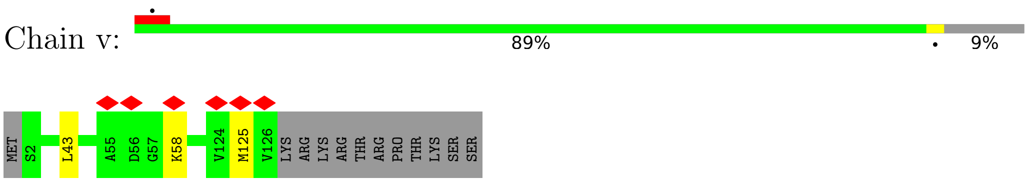
- Molecule 46: 60S ribosomal protein L37a

Chain u:

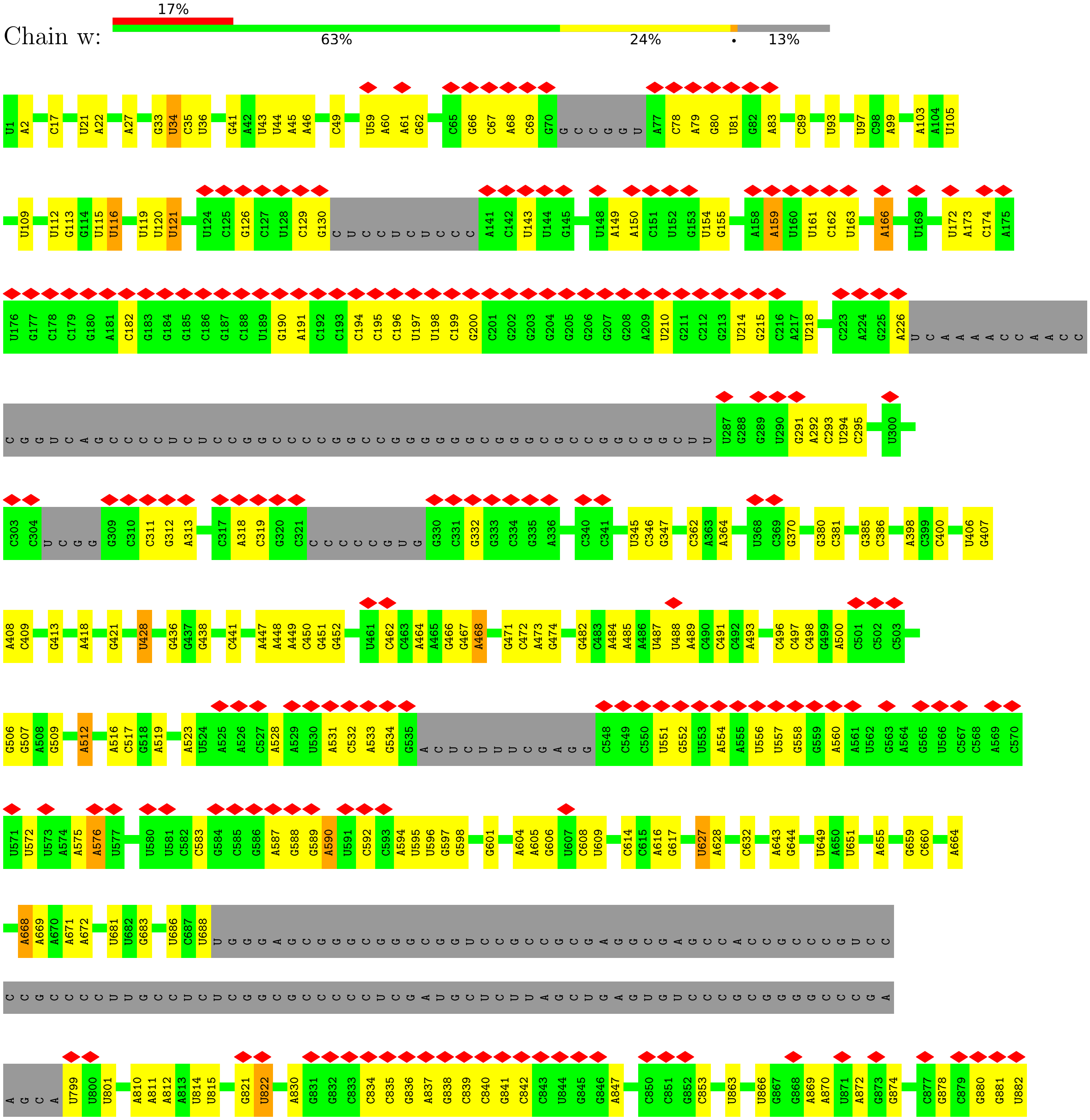


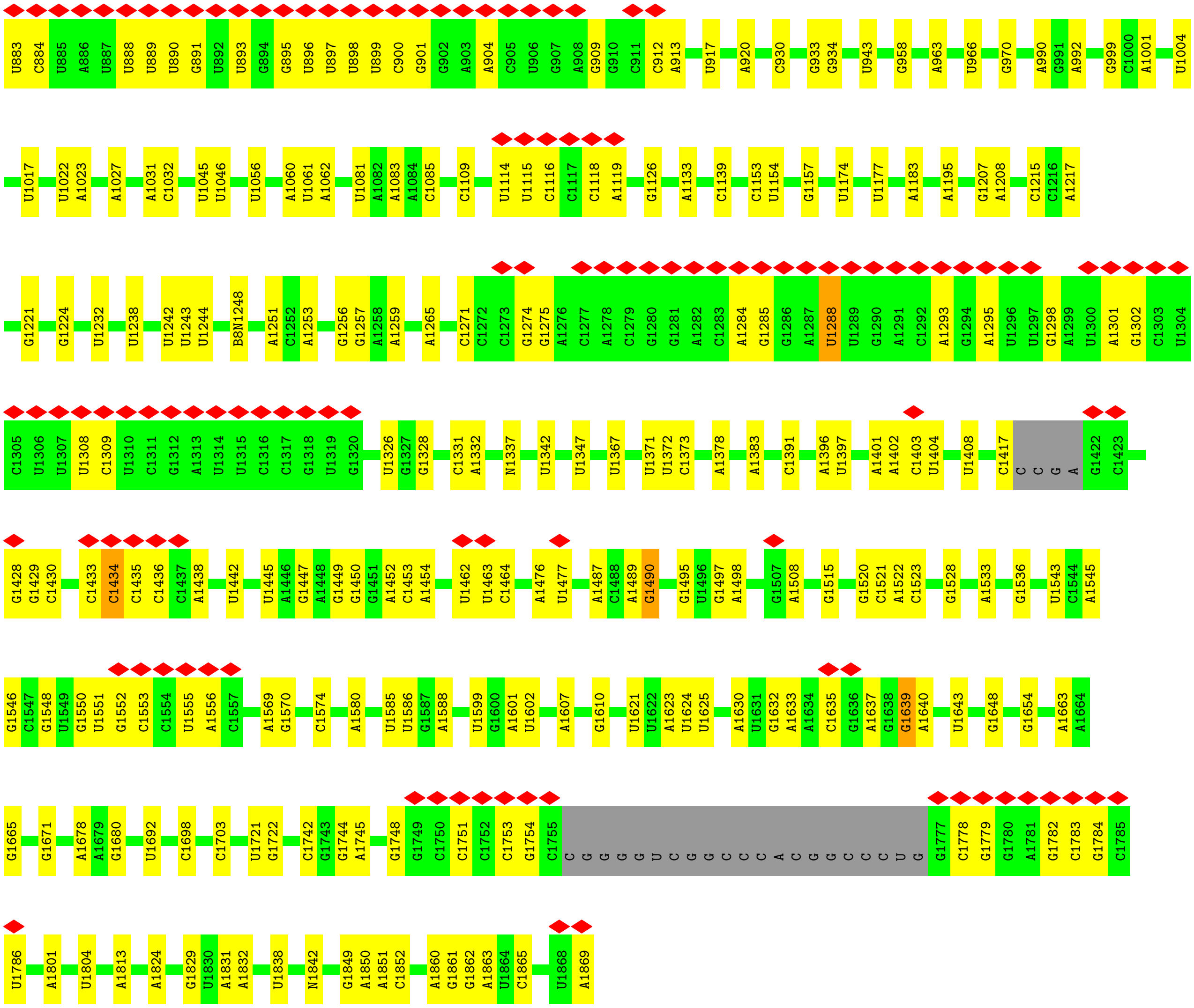


- Molecule 47: 60S ribosomal protein L28



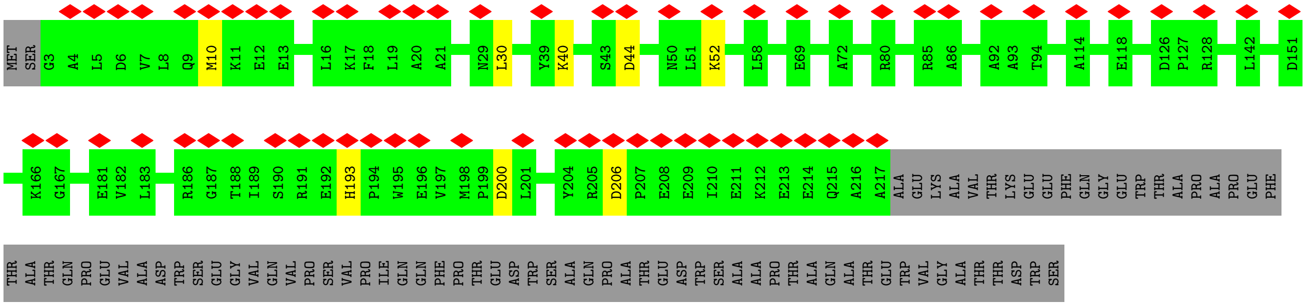
- Molecule 48: 18S ribosomal RNA





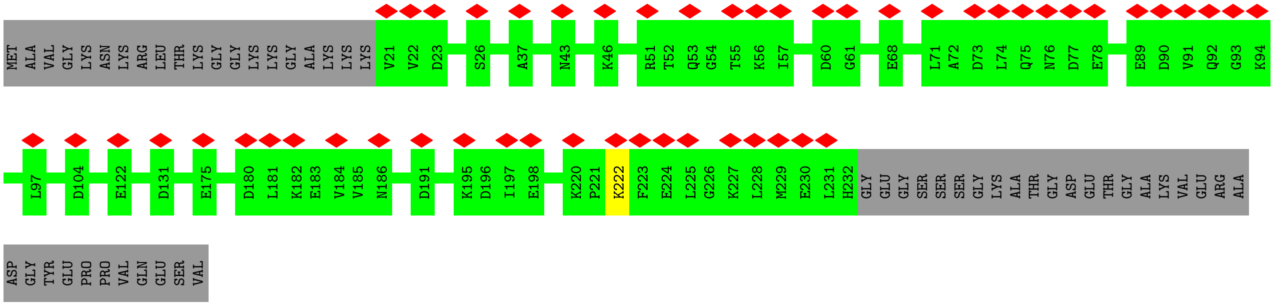
- Molecule 49: 40S ribosomal protein SA

Chain x:



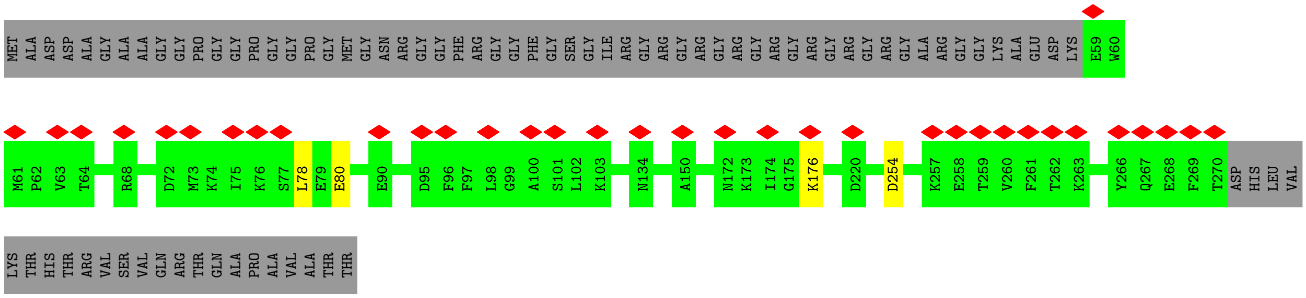
- Molecule 50: 40S ribosomal protein S3a

Chain y:



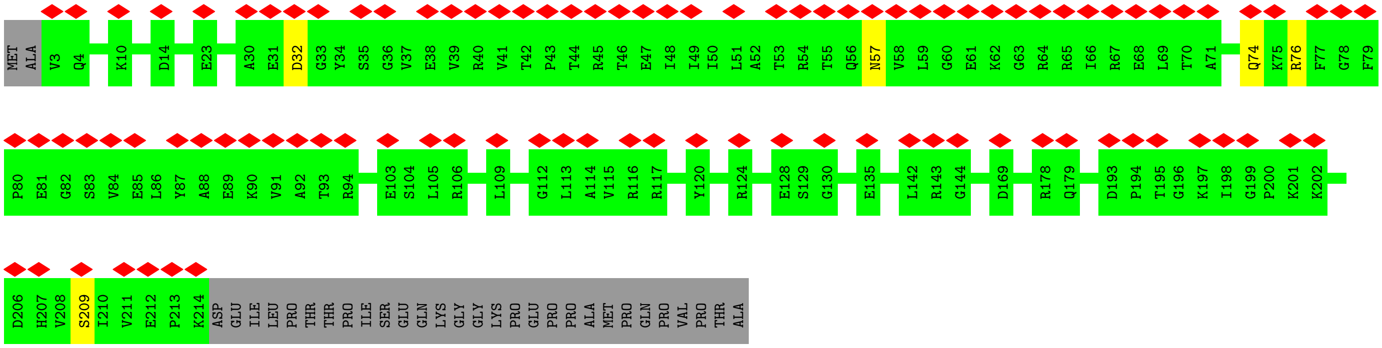
- Molecule 51: 40S ribosomal protein S2

Chain z:



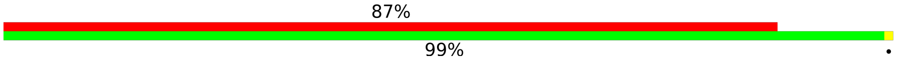
- Molecule 52: 40S ribosomal protein S3

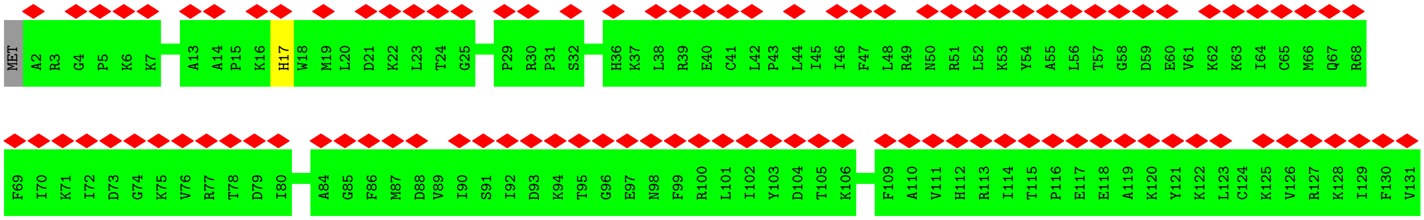
Chain 0:

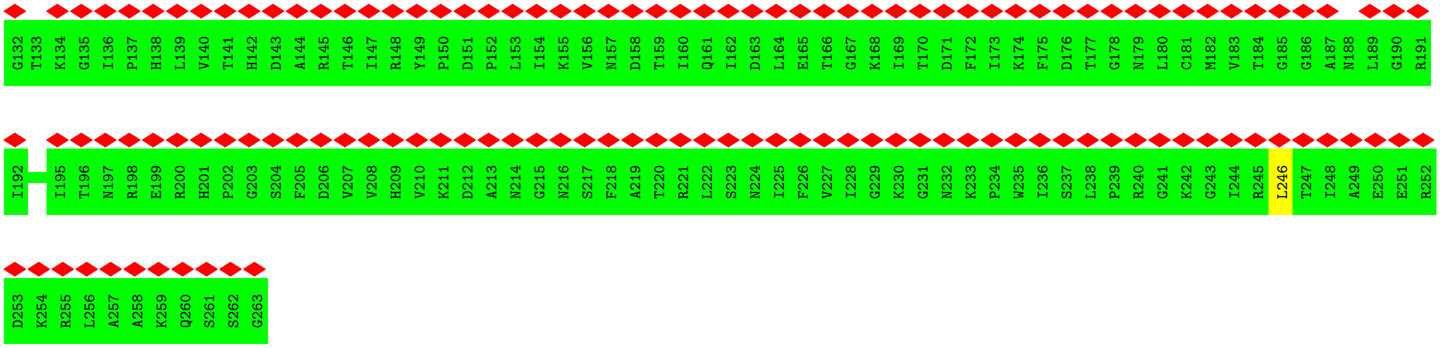


- Molecule 53: 40S ribosomal protein S4, X isoform

Chain 1:

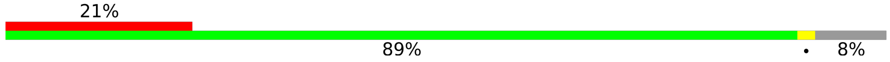


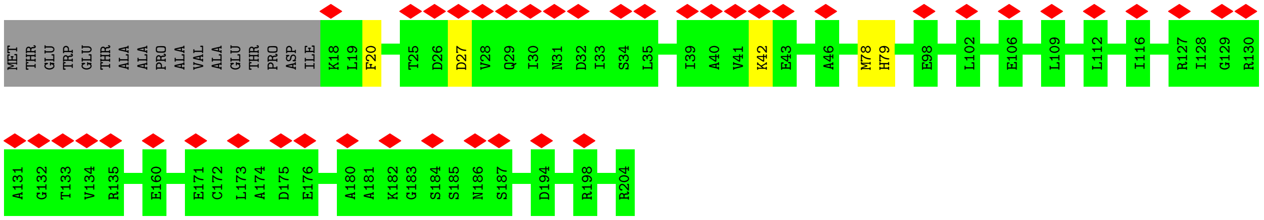




- Molecule 54: 40S ribosomal protein S5

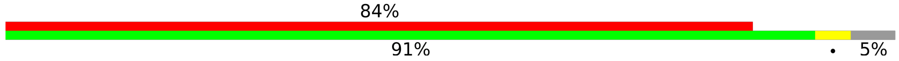
Chain 2:

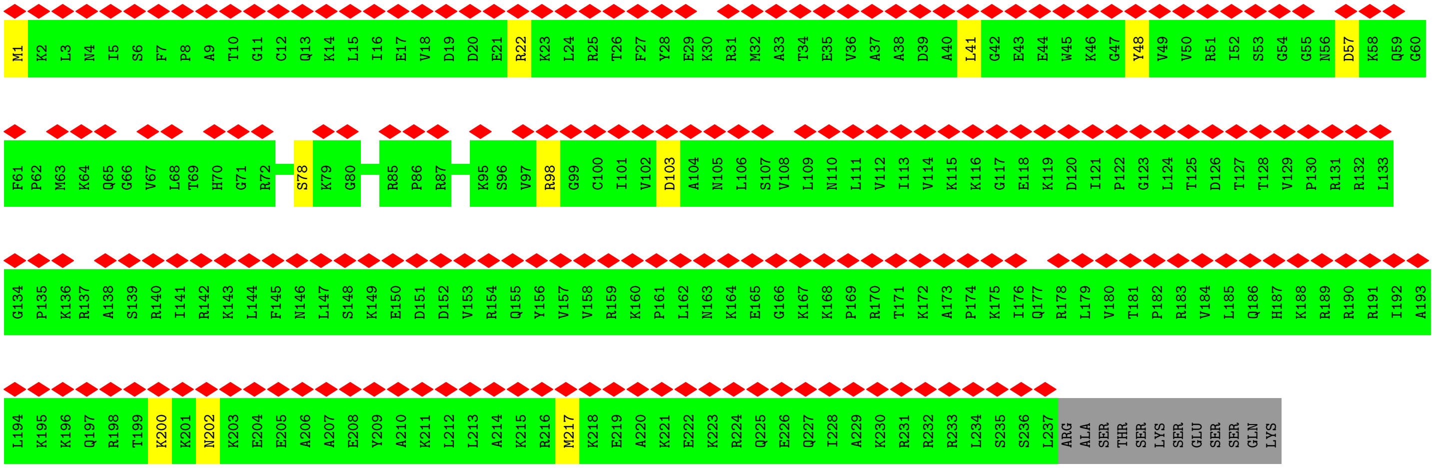




- Molecule 55: 40S ribosomal protein S6

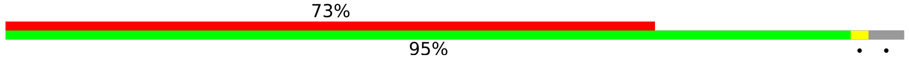
Chain 3:

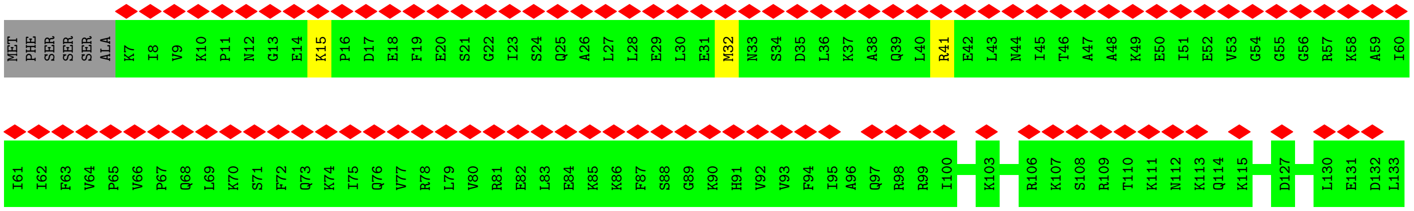


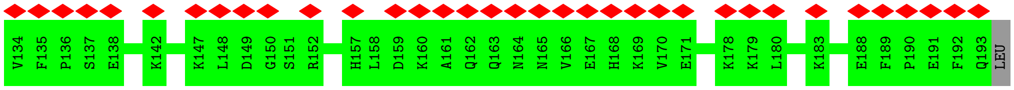


- Molecule 56: 40S ribosomal protein S7

Chain 4:

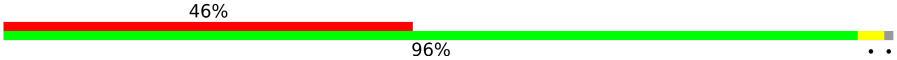


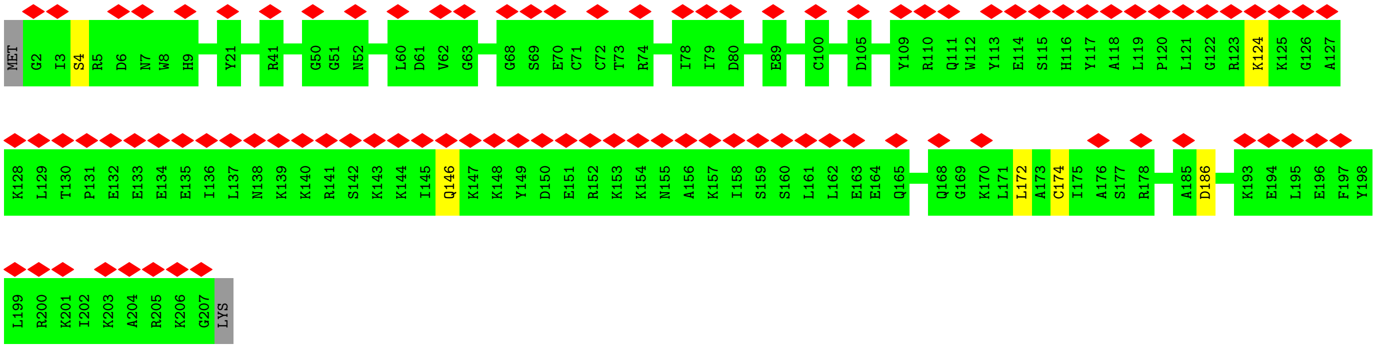




- Molecule 57: 40S ribosomal protein S8

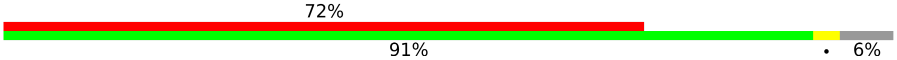
Chain 5:

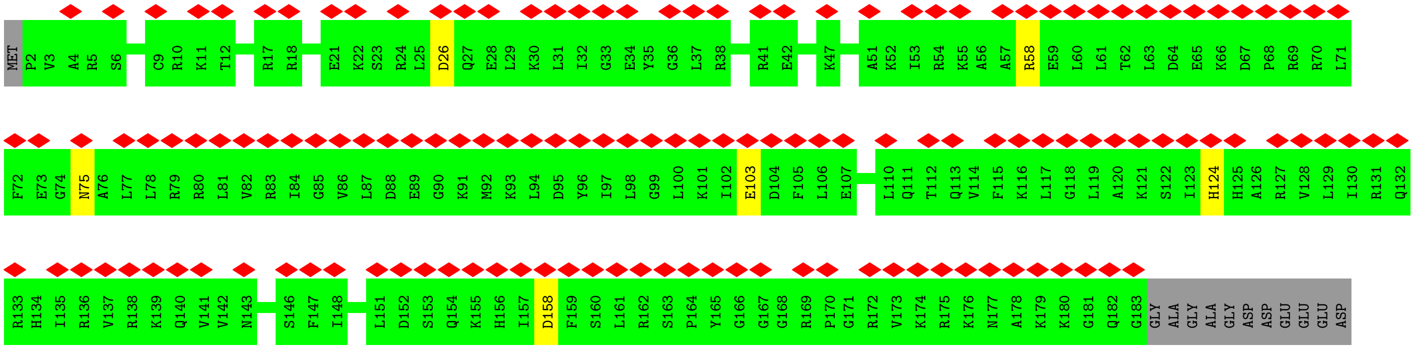




- Molecule 58: 40S ribosomal protein S9

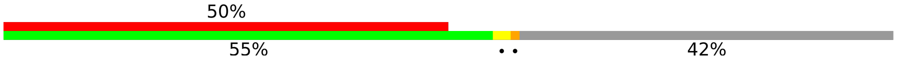
Chain 6:

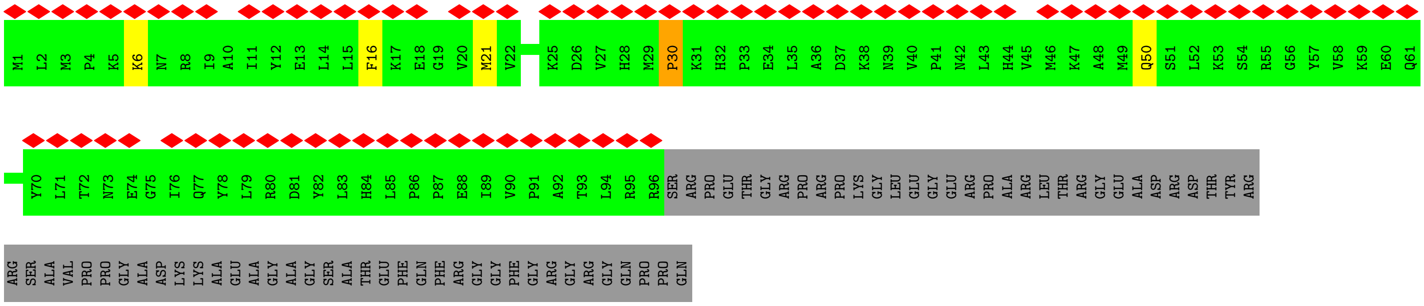




- Molecule 59: 40S ribosomal protein S10

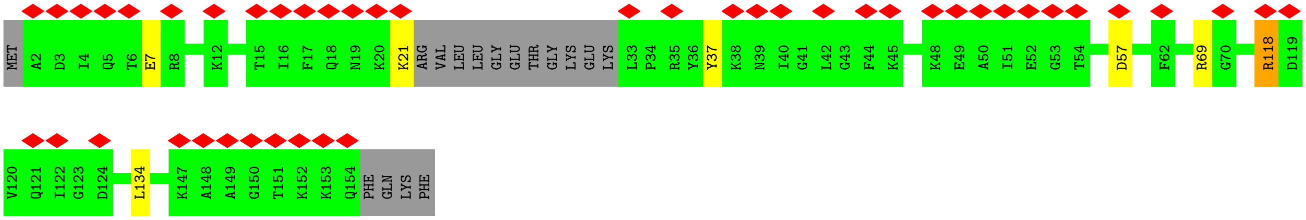
Chain 7:





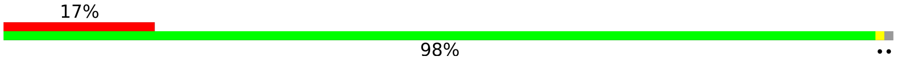
- Molecule 60: 40S ribosomal protein S11

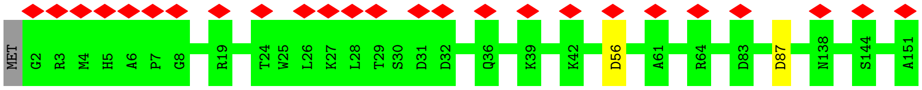
Chain 8:



- Molecule 61: 40S ribosomal protein S13

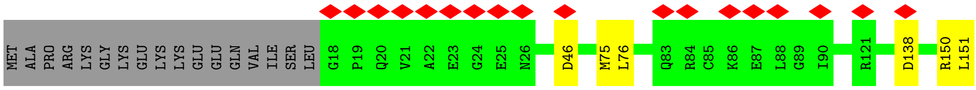
Chain 9:





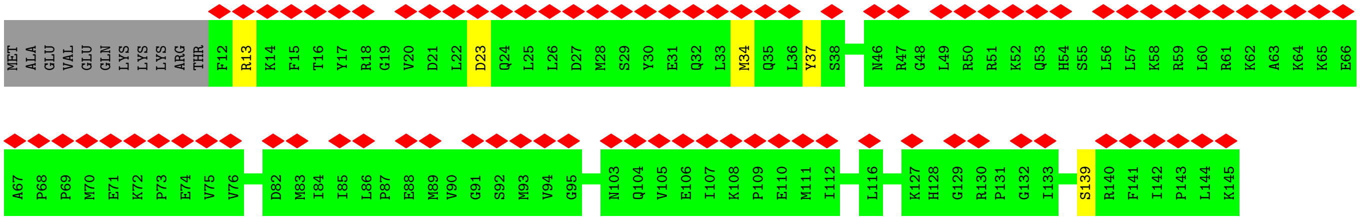
- Molecule 62: 40S ribosomal protein S14

Chain AA:



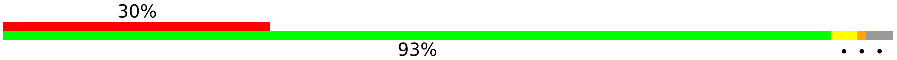
- Molecule 63: 40S ribosomal protein S15

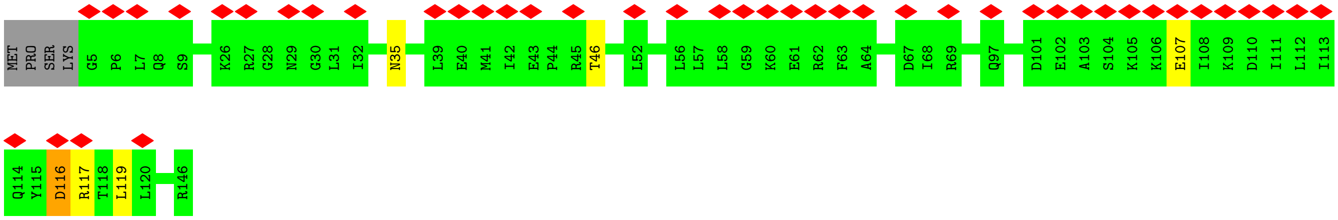
Chain AB:



- Molecule 64: 40S ribosomal protein S16

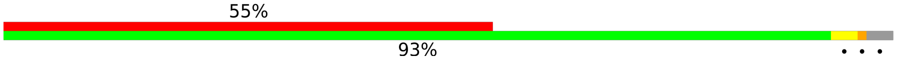
Chain AC:

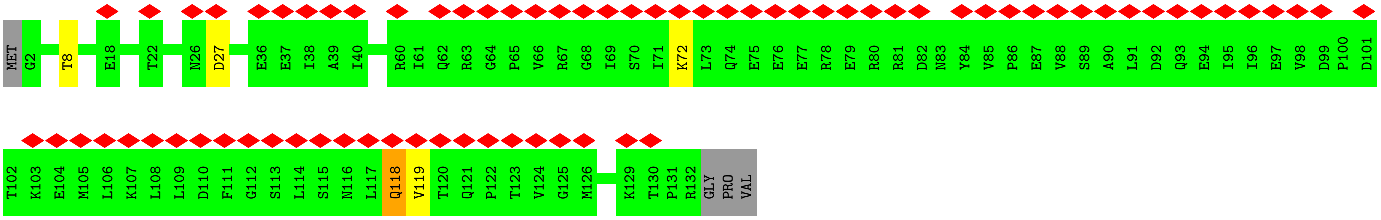




- Molecule 65: 40S ribosomal protein S17

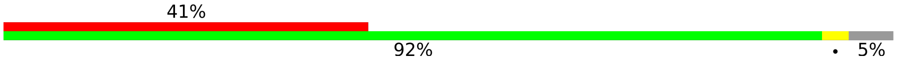
Chain AD:

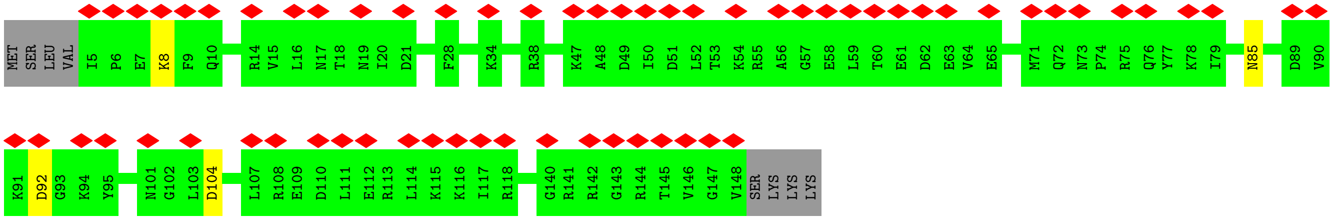




- Molecule 66: 40S ribosomal protein S18

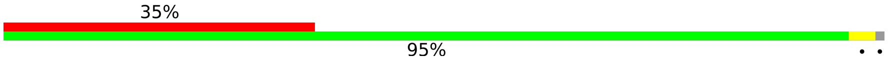
Chain AE:

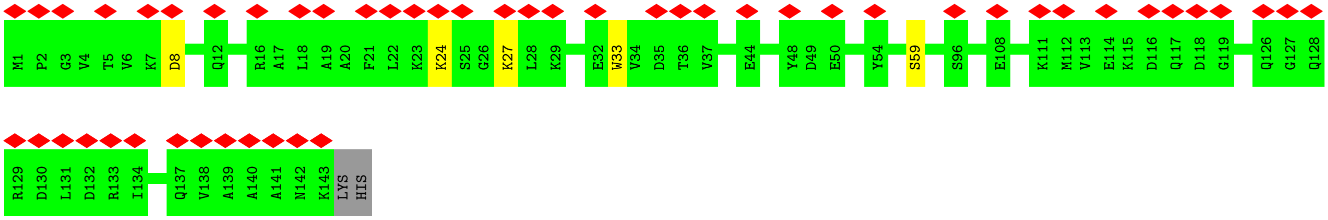




- Molecule 67: 40S ribosomal protein S19

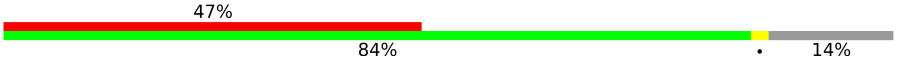
Chain AF:





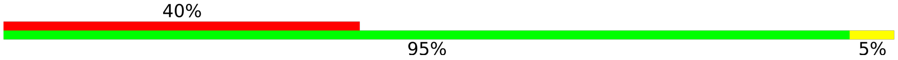
- Molecule 68: 40S ribosomal protein S20

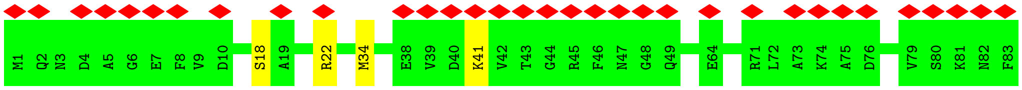
Chain AG:



- Molecule 69: 40S ribosomal protein S21

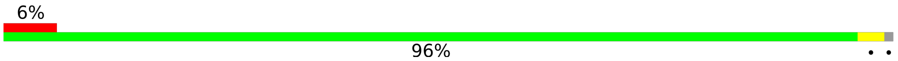
Chain AH:

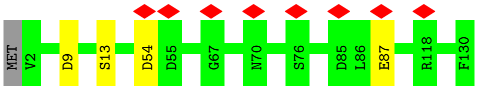




- Molecule 70: 40S ribosomal protein S15a

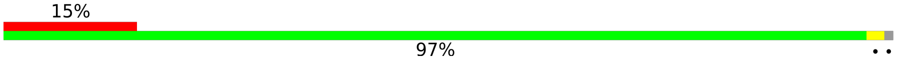
Chain AI:

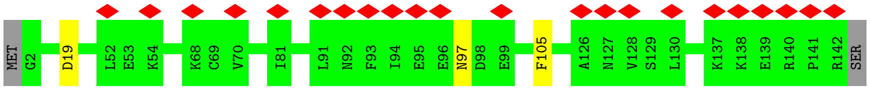




- Molecule 71: 40S ribosomal protein S23

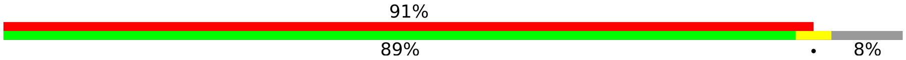
Chain AJ:

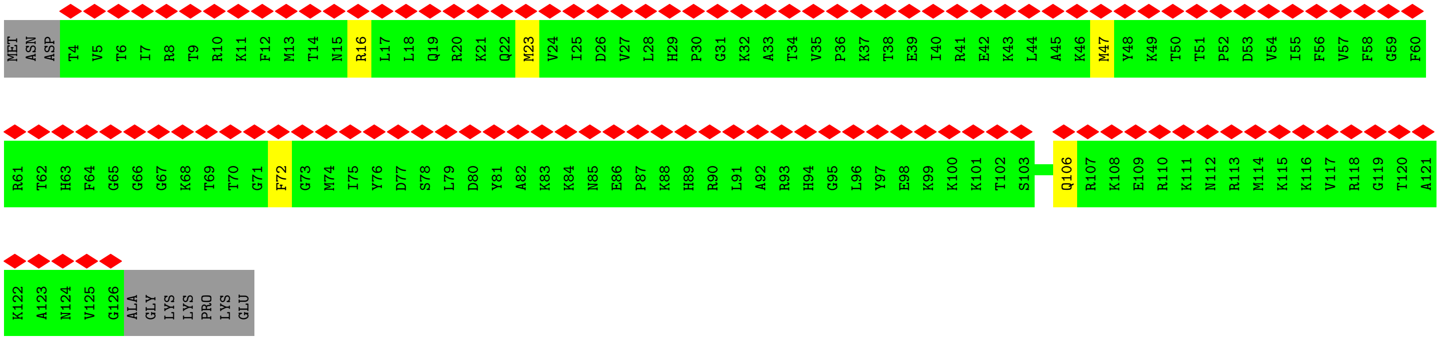




- Molecule 72: 40S ribosomal protein S24

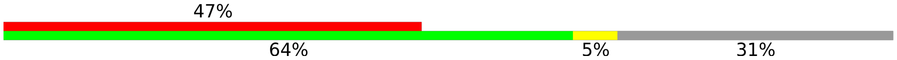
Chain AK:

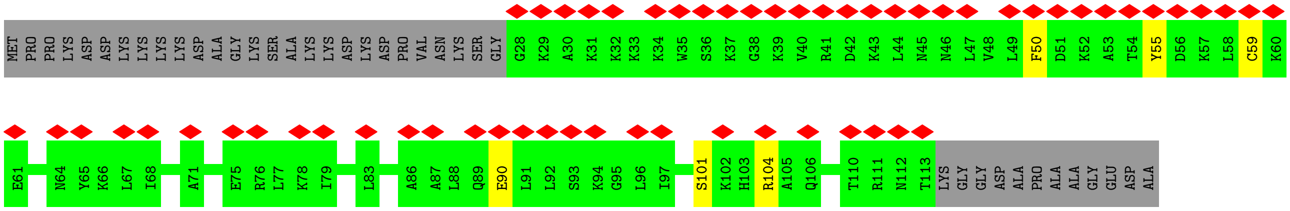




- Molecule 73: 40S ribosomal protein S25

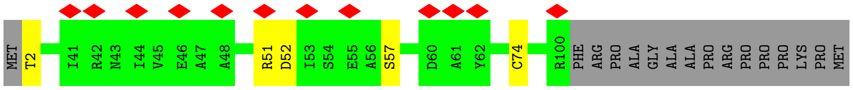
Chain AL:





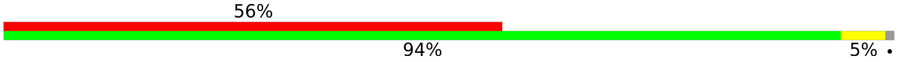
- Molecule 74: 40S ribosomal protein S26

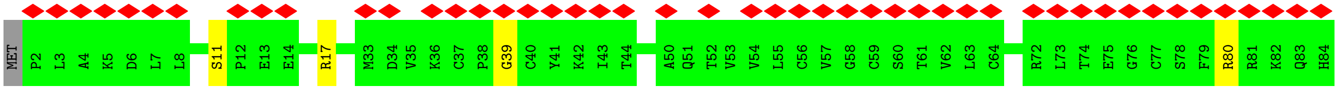
Chain AM:



- Molecule 75: 40S ribosomal protein S27

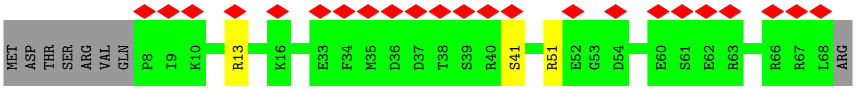
Chain AN:





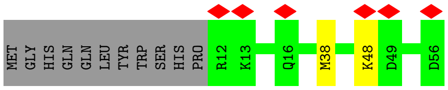
- Molecule 76: 40S ribosomal protein S28

Chain AO:



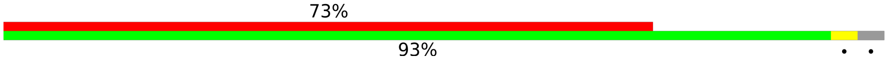
- Molecule 77: 40S ribosomal protein S29

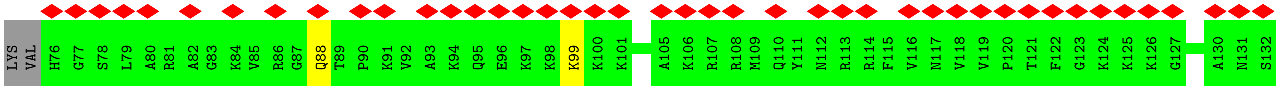
Chain AP:



- Molecule 78: 40S ribosomal protein S30

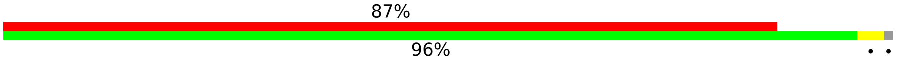
Chain AQ:

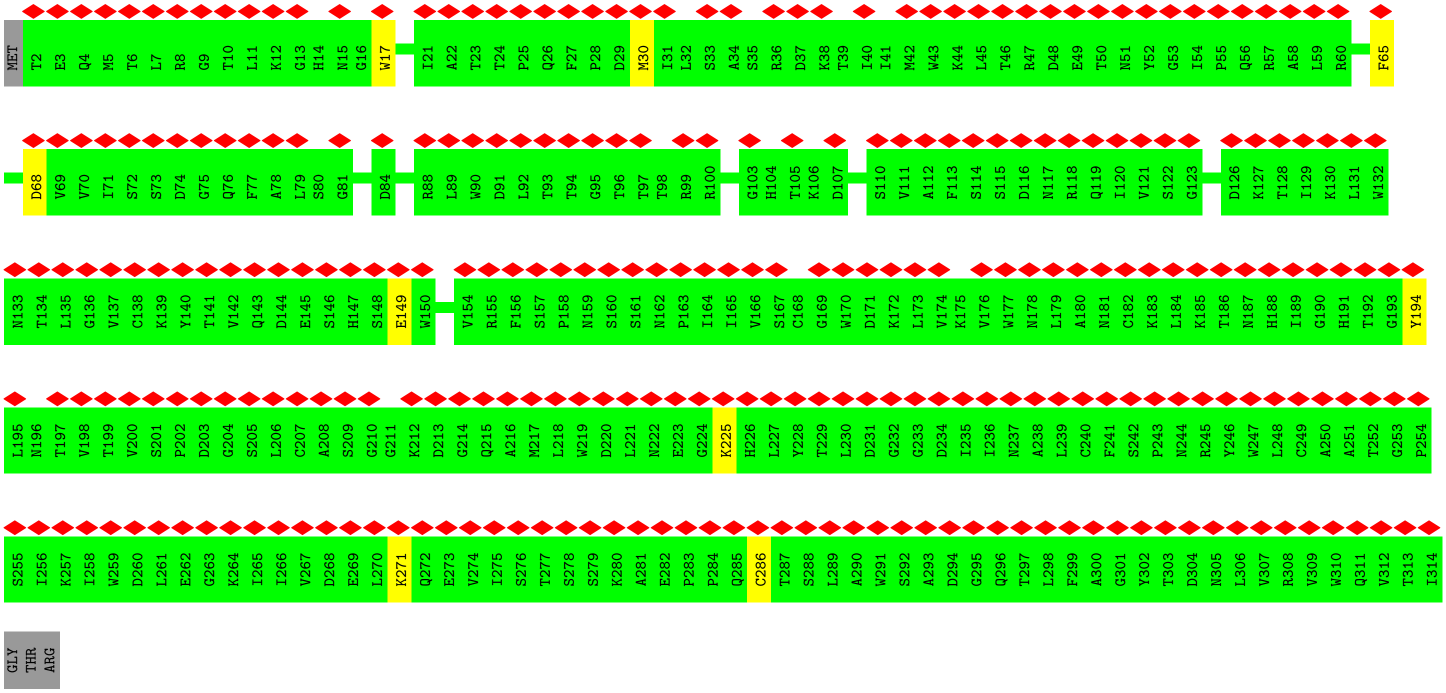




- Molecule 79: Receptor of activated protein C kinase 1

Chain AR:





4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	128240	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 $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0204	Depositor
Map size (Å)	439.9, 439.9, 439.9	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, G7M, OMC, 5MC, 5MU, 1MA, 56B, PSU, ZN, 4AC, MA6, A2M, OMG, 2MG, UY1, 6MZ, H2U, OMU, MG, B8N

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	A	0.43	0/339	0.68	0/527
2	B	0.40	0/1525	0.70	0/2375
2	C	0.30	0/1525	0.72	0/2375
3	D	0.65	0/81567	0.75	17/127232 (0.0%)
4	E	0.66	0/2858	0.71	0/4455
5	F	0.63	0/3675	0.75	4/5725 (0.1%)
6	G	0.38	0/1929	0.52	0/2586
7	H	0.37	0/3279	0.53	2/4388 (0.0%)
8	I	0.35	0/2938	0.50	1/3946 (0.0%)
9	J	0.36	0/2425	0.45	0/3248
10	K	0.32	0/1785	0.49	0/2394
11	L	0.37	0/1905	0.46	0/2539
12	M	0.33	0/1863	0.51	2/2510 (0.1%)
13	N	0.33	0/1537	0.49	0/2066
14	O	0.36	0/1699	0.50	1/2270 (0.0%)
15	P	0.31	0/1385	0.49	0/1852
16	Q	0.34	0/1713	0.47	0/2293
17	R	0.34	0/1142	0.47	0/1527
18	S	0.39	0/1746	0.48	1/2338 (0.0%)
19	T	0.38	0/1673	0.45	0/2238
20	U	0.38	0/1300	0.48	0/1746
21	V	0.38	0/1537	0.52	0/2052
22	W	0.32	0/1524	0.48	0/2013
23	X	0.38	0/1493	0.45	0/2003
24	Y	0.38	0/1326	0.49	0/1770
25	Z	0.31	0/835	0.50	0/1122
26	a	0.37	0/993	0.49	0/1332
27	b	0.36	0/541	0.42	0/720
28	c	0.33	0/998	0.50	0/1340
29	d	0.36	0/1132	0.48	0/1504
30	e	0.37	0/1130	0.48	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	f	0.37	0/1191	0.49	0/1591
32	g	0.30	0/844	0.46	0/1115
33	h	0.35	0/765	0.51	1/1027 (0.1%)
34	i	0.35	0/903	0.47	0/1216
35	j	0.38	0/1071	0.45	0/1429
36	k	0.40	0/895	0.55	0/1198
37	l	0.36	0/898	0.46	0/1197
38	m	0.32	0/1018	0.42	0/1344
39	n	0.30	0/843	0.43	0/1115
40	o	0.38	0/720	0.49	0/952
41	p	0.33	0/575	0.46	0/761
42	q	0.33	0/454	0.42	0/599
43	r	0.34	0/435	0.50	1/575 (0.2%)
44	s	0.31	0/240	0.36	0/305
45	t	0.37	0/876	0.50	0/1156
46	u	0.38	0/718	0.47	0/953
47	v	0.37	0/1017	0.50	0/1364
48	w	0.43	0/37158	0.75	13/57908 (0.0%)
49	x	0.28	0/1732	0.49	1/2355 (0.0%)
50	y	0.28	0/1752	0.48	0/2345
51	z	0.31	0/1668	0.49	0/2254
52	0	0.28	0/1672	0.47	0/2250
53	1	0.25	0/2112	0.46	0/2842
54	2	0.28	0/1485	0.47	0/1998
55	3	0.26	0/1940	0.50	0/2583
56	4	0.27	0/1533	0.52	0/2053
57	5	0.26	0/1703	0.48	1/2275 (0.0%)
58	6	0.25	0/1531	0.44	0/2045
59	7	0.32	0/834	0.64	2/1125 (0.2%)
60	8	0.30	0/1170	0.51	0/1568
61	9	0.27	0/1232	0.47	0/1656
62	AA	0.30	0/1015	0.53	1/1361 (0.1%)
63	AB	0.29	0/1126	0.50	0/1505
64	AC	0.31	0/1146	0.54	1/1534 (0.1%)
65	AD	0.27	0/1071	0.50	0/1438
66	AE	0.31	0/1187	0.58	0/1593
67	AF	0.29	0/1130	0.49	0/1515
68	AG	0.26	0/809	0.50	0/1087
69	AH	0.30	0/643	0.57	0/860
70	AI	0.29	0/1051	0.47	0/1406
71	AJ	0.27	0/1116	0.46	0/1490
72	AK	0.26	0/1019	0.54	0/1355
73	AL	0.26	0/688	0.50	0/921

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
74	AM	0.33	0/805	0.46	0/1079
75	AN	0.28	0/657	0.52	0/883
76	AO	0.28	0/481	0.61	0/643
77	AP	0.35	0/375	0.55	0/492
78	AQ	0.28	0/458	0.48	0/602
79	AR	0.26	0/2493	0.54	2/3394 (0.1%)
All	All	0.50	0/219572	0.66	51/322305 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	G	0	2
7	H	0	2
8	I	0	1
9	J	0	1
10	K	0	1
11	L	0	1
16	Q	0	1
20	U	0	1
21	V	0	1
24	Y	0	1
29	d	0	1
32	g	0	1
40	o	0	1
54	2	0	1
65	AD	0	1
79	AR	0	1
All	All	0	18

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2101	C	O5'-P-OP1	-27.25	78.00	110.70
3	D	2101	C	OP1-P-OP2	-26.57	79.75	119.60
3	D	2101	C	O5'-P-OP2	16.09	130.01	110.70
3	D	2100	A	OP2-P-O3'	-15.46	71.19	105.20
3	D	2100	A	OP1-P-O3'	14.11	136.24	105.20
59	7	30	PRO	CA-N-CD	-12.34	94.22	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	316	LYS	C-N-CA	-8.40	100.71	121.70
48	w	1453	C	C2-N1-C1’	8.25	127.87	118.80
48	w	1453	C	N1-C2-O2	7.77	123.56	118.90
18	S	135	ILE	C-N-CA	-7.49	102.97	121.70
5	F	110	U	C2-N1-C1’	7.42	126.61	117.70
5	F	110	U	N1-C2-O2	7.07	127.75	122.80
3	D	233	U	N1-C2-O2	6.81	127.56	122.80
5	F	110	U	N3-C2-O2	-6.80	117.44	122.20
3	D	233	U	N3-C2-O2	-6.72	117.50	122.20
3	D	2409	U	C2-N1-C1’	6.21	125.15	117.70
48	w	1520	G	C4-N9-C1’	6.14	134.49	126.50
48	w	1453	C	N3-C2-O2	-6.04	117.67	121.90
48	w	1453	C	C6-N1-C1’	-5.87	113.76	120.80
3	D	209	U	C2-N1-C1’	5.86	124.73	117.70
3	D	233	U	C2-N1-C1’	5.61	124.43	117.70
3	D	3775	A	O4’-C1’-N9	5.58	112.66	108.20
12	M	206	GLN	CA-CB-CG	5.50	125.50	113.40
43	r	78	ILE	C-N-CA	-5.45	108.09	121.70
49	x	206	ASP	CB-CG-OD1	5.44	123.19	118.30
3	D	1241	C	C2-N1-C1’	5.40	124.74	118.80
14	O	193	ASP	CB-CG-OD2	5.40	123.16	118.30
64	AC	116	ASP	CB-CG-OD1	5.37	123.13	118.30
3	D	2675	G	P-O3’-C3’	5.36	126.13	119.70
79	AR	30	MET	CB-CG-SD	5.36	128.47	112.40
59	7	30	PRO	N-CD-CG	-5.35	95.18	103.20
7	H	360	LEU	CA-CB-CG	5.34	127.59	115.30
57	5	172	LEU	CA-CB-CG	5.30	127.50	115.30
33	h	20	LEU	CA-CB-CG	5.30	127.49	115.30
48	w	1331	C	P-O3’-C3’	5.29	126.05	119.70
3	D	417	G	O4’-C1’-N9	5.28	112.42	108.20
62	AA	76	LEU	CA-CB-CG	5.26	127.40	115.30
48	w	1022	U	C2-N1-C1’	5.25	124.00	117.70
79	AR	30	MET	CA-CB-CG	5.21	122.16	113.30
48	w	1520	G	C8-N9-C1’	-5.18	120.27	127.00
48	w	1434	C	C2-N1-C1’	5.17	124.49	118.80
48	w	1434	C	N1-C2-O2	5.17	122.00	118.90
7	H	309	LEU	CA-CB-CG	5.17	127.18	115.30
5	F	111	U	C2-N1-C1’	5.16	123.89	117.70
12	M	115	LEU	CA-CB-CG	5.15	127.15	115.30
48	w	1139	C	C2-N1-C1’	5.13	124.45	118.80
3	D	2409	U	N1-C2-O2	5.12	126.38	122.80
3	D	4348	A	OP1-P-O3’	5.06	116.33	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	4348	A	P-O3'-C3'	5.03	125.74	119.70
48	w	1453	C	C6-N1-C2	-5.03	118.29	120.30
48	w	1860	A	P-O3'-C3'	5.02	125.73	119.70

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	2	79	HIS	Peptide
65	AD	118	GLN	Peptide
79	AR	149	GLU	Peptide
6	G	123	ARG	Peptide
6	G	239	ALA	Peptide
7	H	16	PHE	Peptide
7	H	258	HIS	Peptide
8	I	91	ALA	Peptide
9	J	124	GLU	Peptide
10	K	130	LYS	Peptide
11	L	163	ASN	Peptide
16	Q	47	ALA	Peptide
20	U	131	ARG	Peptide
21	V	159	PRO	Peptide
24	Y	80	VAL	Peptide
29	d	108	ARG	Peptide
32	g	110	ALA	Peptide
40	o	39	TYR	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	245/257 (95%)	227 (93%)	18 (7%)	0	100	100
7	H	396/403 (98%)	375 (95%)	21 (5%)	0	100	100
8	I	361/427 (84%)	338 (94%)	23 (6%)	0	100	100
9	J	291/297 (98%)	271 (93%)	20 (7%)	0	100	100
10	K	211/288 (73%)	189 (90%)	22 (10%)	0	100	100
11	L	223/248 (90%)	212 (95%)	11 (5%)	0	100	100
12	M	223/266 (84%)	208 (93%)	14 (6%)	1 (0%)	34	54
13	N	188/192 (98%)	174 (93%)	14 (7%)	0	100	100
14	O	202/214 (94%)	186 (92%)	16 (8%)	0	100	100
15	P	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
16	Q	206/211 (98%)	192 (93%)	12 (6%)	2 (1%)	15	28
17	R	134/215 (62%)	120 (90%)	14 (10%)	0	100	100
18	S	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
19	T	198/203 (98%)	195 (98%)	3 (2%)	0	100	100
20	U	155/184 (84%)	144 (93%)	11 (7%)	0	100	100
21	V	185/188 (98%)	173 (94%)	12 (6%)	0	100	100
22	W	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
23	X	173/176 (98%)	159 (92%)	14 (8%)	0	100	100
24	Y	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
25	Z	99/128 (77%)	93 (94%)	6 (6%)	0	100	100
26	a	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
27	b	61/157 (39%)	60 (98%)	1 (2%)	0	100	100
28	c	118/156 (76%)	111 (94%)	7 (6%)	0	100	100
29	d	132/145 (91%)	125 (95%)	7 (5%)	0	100	100
30	e	133/136 (98%)	126 (95%)	6 (4%)	1 (1%)	19	35
31	f	145/148 (98%)	131 (90%)	14 (10%)	0	100	100
32	g	100/159 (63%)	90 (90%)	8 (8%)	2 (2%)	7	12
33	h	95/115 (83%)	91 (96%)	4 (4%)	0	100	100
34	i	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
35	j	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
36	k	107/110 (97%)	99 (92%)	8 (8%)	0	100	100
37	l	110/117 (94%)	106 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	m	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
39	n	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
40	o	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
41	p	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
42	q	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	r	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
44	s	23/25 (92%)	23 (100%)	0	0	100	100
45	t	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
46	u	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
47	v	123/137 (90%)	116 (94%)	7 (6%)	0	100	100
49	x	213/295 (72%)	200 (94%)	13 (6%)	0	100	100
50	y	210/264 (80%)	193 (92%)	17 (8%)	0	100	100
51	z	210/293 (72%)	200 (95%)	9 (4%)	1 (0%)	29	48
52	0	210/243 (86%)	188 (90%)	22 (10%)	0	100	100
53	1	260/263 (99%)	245 (94%)	15 (6%)	0	100	100
54	2	185/204 (91%)	166 (90%)	19 (10%)	0	100	100
55	3	235/249 (94%)	226 (96%)	9 (4%)	0	100	100
56	4	185/194 (95%)	168 (91%)	17 (9%)	0	100	100
57	5	204/208 (98%)	192 (94%)	12 (6%)	0	100	100
58	6	180/194 (93%)	171 (95%)	9 (5%)	0	100	100
59	7	94/165 (57%)	86 (92%)	7 (7%)	1 (1%)	14	26
60	8	138/158 (87%)	126 (91%)	11 (8%)	1 (1%)	22	39
61	9	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
62	AA	132/151 (87%)	123 (93%)	9 (7%)	0	100	100
63	AB	132/145 (91%)	126 (96%)	6 (4%)	0	100	100
64	AC	140/146 (96%)	124 (89%)	15 (11%)	1 (1%)	22	39
65	AD	129/135 (96%)	107 (83%)	20 (16%)	2 (2%)	9	17
66	AE	142/152 (93%)	128 (90%)	14 (10%)	0	100	100
67	AF	141/145 (97%)	132 (94%)	9 (6%)	0	100	100
68	AG	100/119 (84%)	92 (92%)	8 (8%)	0	100	100
69	AH	81/83 (98%)	72 (89%)	9 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	AI	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
71	AJ	139/143 (97%)	135 (97%)	4 (3%)	0	100	100
72	AK	121/133 (91%)	118 (98%)	3 (2%)	0	100	100
73	AL	84/125 (67%)	74 (88%)	10 (12%)	0	100	100
74	AM	97/115 (84%)	91 (94%)	6 (6%)	0	100	100
75	AN	81/84 (96%)	71 (88%)	9 (11%)	1 (1%)	13	24
76	AO	59/69 (86%)	53 (90%)	6 (10%)	0	100	100
77	AP	43/56 (77%)	42 (98%)	1 (2%)	0	100	100
78	AQ	55/59 (93%)	50 (91%)	5 (9%)	0	100	100
79	AR	311/317 (98%)	261 (84%)	50 (16%)	0	100	100
All	All	10947/12400 (88%)	10208 (93%)	726 (7%)	13 (0%)	54	73

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	48	PRO
32	g	111	ARG
64	AC	119	LEU
51	z	78	LEU
65	AD	119	VAL
32	g	110	ALA
65	AD	118	GLN
16	Q	47	ALA
30	e	33	THR
12	M	106	THR
60	8	118	ARG
59	7	30	PRO
75	AN	39	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	189/199 (95%)	189 (100%)	0	100	100
7	H	346/349 (99%)	341 (99%)	5 (1%)	67	86
8	I	301/348 (86%)	294 (98%)	7 (2%)	50	76
9	J	245/250 (98%)	241 (98%)	4 (2%)	62	84
10	K	193/252 (77%)	189 (98%)	4 (2%)	53	78
11	L	194/215 (90%)	192 (99%)	2 (1%)	76	90
12	M	195/223 (87%)	192 (98%)	3 (2%)	65	85
13	N	169/171 (99%)	166 (98%)	3 (2%)	59	81
14	O	174/181 (96%)	171 (98%)	3 (2%)	60	82
15	P	143/149 (96%)	139 (97%)	4 (3%)	43	70
16	Q	174/177 (98%)	172 (99%)	2 (1%)	73	89
17	R	116/161 (72%)	112 (97%)	4 (3%)	37	63
18	S	171/172 (99%)	168 (98%)	3 (2%)	59	81
19	T	172/174 (99%)	167 (97%)	5 (3%)	42	69
20	U	138/163 (85%)	135 (98%)	3 (2%)	52	77
21	V	164/165 (99%)	164 (100%)	0	100	100
22	W	159/175 (91%)	158 (99%)	1 (1%)	86	95
23	X	156/157 (99%)	156 (100%)	0	100	100
24	Y	139/140 (99%)	134 (96%)	5 (4%)	35	61
25	Z	90/115 (78%)	84 (93%)	6 (7%)	16	31
26	a	101/107 (94%)	99 (98%)	2 (2%)	55	79
27	b	55/126 (44%)	54 (98%)	1 (2%)	59	81
28	c	107/133 (80%)	105 (98%)	2 (2%)	57	80
29	d	124/135 (92%)	121 (98%)	3 (2%)	49	74
30	e	117/118 (99%)	112 (96%)	5 (4%)	29	53
31	f	120/121 (99%)	119 (99%)	1 (1%)	81	93
32	g	81/126 (64%)	76 (94%)	5 (6%)	18	35
33	h	82/97 (84%)	80 (98%)	2 (2%)	49	74
34	i	98/110 (89%)	95 (97%)	3 (3%)	40	67
35	j	114/121 (94%)	113 (99%)	1 (1%)	78	92
36	k	88/89 (99%)	88 (100%)	0	100	100
37	l	96/100 (96%)	95 (99%)	1 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	m	109/110 (99%)	109 (100%)	0	100	100
39	n	86/89 (97%)	85 (99%)	1 (1%)	71	88
40	o	73/80 (91%)	72 (99%)	1 (1%)	67	86
41	p	64/65 (98%)	63 (98%)	1 (2%)	62	84
42	q	47/48 (98%)	44 (94%)	3 (6%)	17	33
43	r	48/116 (41%)	47 (98%)	1 (2%)	53	78
44	s	24/24 (100%)	23 (96%)	1 (4%)	30	54
45	t	93/94 (99%)	91 (98%)	2 (2%)	52	77
46	u	74/75 (99%)	74 (100%)	0	100	100
47	v	109/121 (90%)	106 (97%)	3 (3%)	43	70
49	x	178/243 (73%)	171 (96%)	7 (4%)	32	57
50	y	194/231 (84%)	193 (100%)	1 (0%)	88	96
51	z	176/225 (78%)	173 (98%)	3 (2%)	60	82
52	0	175/202 (87%)	170 (97%)	5 (3%)	42	69
53	1	223/225 (99%)	221 (99%)	2 (1%)	78	92
54	2	154/170 (91%)	150 (97%)	4 (3%)	46	72
55	3	206/218 (94%)	195 (95%)	11 (5%)	22	43
56	4	168/174 (97%)	165 (98%)	3 (2%)	59	81
57	5	175/180 (97%)	170 (97%)	5 (3%)	42	69
58	6	160/168 (95%)	154 (96%)	6 (4%)	33	58
59	7	87/136 (64%)	83 (95%)	4 (5%)	27	50
60	8	125/142 (88%)	118 (94%)	7 (6%)	21	40
61	9	130/131 (99%)	128 (98%)	2 (2%)	65	85
62	AA	104/119 (87%)	99 (95%)	5 (5%)	25	48
63	AB	120/130 (92%)	115 (96%)	5 (4%)	30	54
64	AC	117/121 (97%)	112 (96%)	5 (4%)	29	53
65	AD	117/122 (96%)	114 (97%)	3 (3%)	46	72
66	AE	119/132 (90%)	115 (97%)	4 (3%)	37	63
67	AF	113/115 (98%)	108 (96%)	5 (4%)	28	52
68	AG	89/107 (83%)	87 (98%)	2 (2%)	52	77
69	AH	67/67 (100%)	63 (94%)	4 (6%)	19	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	AI	112/113 (99%)	108 (96%)	4 (4%)	35	61
71	AJ	113/115 (98%)	110 (97%)	3 (3%)	44	71
72	AK	106/115 (92%)	101 (95%)	5 (5%)	26	49
73	AL	73/103 (71%)	67 (92%)	6 (8%)	11	22
74	AM	86/98 (88%)	81 (94%)	5 (6%)	20	38
75	AN	73/76 (96%)	70 (96%)	3 (4%)	30	55
76	AO	54/62 (87%)	51 (94%)	3 (6%)	21	40
77	AP	39/49 (80%)	37 (95%)	2 (5%)	24	45
78	AQ	46/48 (96%)	44 (96%)	2 (4%)	29	53
79	AR	272/275 (99%)	265 (97%)	7 (3%)	46	72
All	All	9509/10553 (90%)	9273 (98%)	236 (2%)	50	73

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	10	ARG
7	H	141	ASP
7	H	289	GLN
7	H	300	LYS
7	H	358	ARG
8	I	71	ARG
8	I	95	MET
8	I	111	TRP
8	I	188	ARG
8	I	212	ASN
8	I	312	ARG
8	I	325	MET
9	J	131	ASN
9	J	256	LYS
9	J	270	LYS
9	J	291	GLN
10	K	50	LEU
10	K	56	ARG
10	K	158	ARG
10	K	251	LYS
11	L	34	ARG
11	L	232	ASP
12	M	115	LEU

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Mol	Chain	Res	Type
12	M	220	GLU
12	M	231	ASP
13	N	36	ARG
13	N	66	GLU
13	N	177	ASP
14	O	123	GLN
14	O	162	ARG
14	O	213	HIS
15	P	8	LYS
15	P	112	HIS
15	P	134	LEU
15	P	148	THR
16	Q	130	LYS
16	Q	162	LYS
17	R	67	SER
17	R	96	GLU
17	R	99	GLU
17	R	108	ASP
18	S	136	ASP
18	S	159	ARG
18	S	174	LEU
19	T	5	GLN
19	T	87	MET
19	T	106	ASP
19	T	117	ARG
19	T	162	GLU
20	U	13	LYS
20	U	20	SER
20	U	21	ASN
22	W	162	ARG
24	Y	41	ASP
24	Y	52	MET
24	Y	79	GLN
24	Y	118	GLU
24	Y	137	GLU
25	Z	24	ASP
25	Z	39	PHE
25	Z	41	GLN
25	Z	65	ARG
25	Z	98	ASP
25	Z	109	SER
26	a	48	ARG

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Mol	Chain	Res	Type
26	a	71	GLU
27	b	1	MET
28	c	67	ARG
28	c	115	LYS
29	d	66	GLN
29	d	108	ARG
29	d	111	LEU
30	e	30	ASP
30	e	34	SER
30	e	35	ASP
30	e	99	ASP
30	e	102	ARG
31	f	140	VAL
32	g	11	ASN
32	g	55	LYS
32	g	58	GLN
32	g	63	LYS
32	g	94	ASP
33	h	20	LEU
33	h	26	LYS
34	i	22	THR
34	i	54	MET
34	i	98	SER
35	j	33	ARG
37	l	65	MET
39	n	66	ASP
40	o	48	ASN
41	p	28	ASN
42	q	8	ARG
42	q	16	LYS
42	q	51	LEU
43	r	113	LYS
44	s	16	LYS
45	t	59	LYS
45	t	74	GLU
47	v	43	LEU
47	v	58	LYS
47	v	125	MET
49	x	10	MET
49	x	30	LEU
49	x	40	LYS
49	x	44	ASP

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Mol	Chain	Res	Type
49	x	52	LYS
49	x	193	HIS
49	x	200	ASP
50	y	222	LYS
51	z	80	GLU
51	z	176	LYS
51	z	254	ASP
52	0	32	ASP
52	0	57	ASN
52	0	74	GLN
52	0	76	ARG
52	0	209	SER
53	1	17	HIS
53	1	246	LEU
54	2	20	PHE
54	2	27	ASP
54	2	42	LYS
54	2	78	MET
55	3	1	MET
55	3	22	ARG
55	3	41	LEU
55	3	48	TYR
55	3	57	ASP
55	3	78	SER
55	3	98	ARG
55	3	103	ASP
55	3	200	LYS
55	3	202	ASN
55	3	217	MET
56	4	15	LYS
56	4	32	MET
56	4	41	ARG
57	5	4	SER
57	5	124	LYS
57	5	146	GLN
57	5	174	CYS
57	5	186	ASP
58	6	26	ASP
58	6	58	ARG
58	6	75	ASN
58	6	103	GLU
58	6	124	HIS

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Mol	Chain	Res	Type
58	6	158	ASP
59	7	6	LYS
59	7	16	PHE
59	7	21	MET
59	7	50	GLN
60	8	7	GLU
60	8	21	LYS
60	8	37	TYR
60	8	57	ASP
60	8	69	ARG
60	8	118	ARG
60	8	134	LEU
61	9	56	ASP
61	9	87	ASP
62	AA	46	ASP
62	AA	75	MET
62	AA	138	ASP
62	AA	150	ARG
62	AA	151	LEU
63	AB	13	ARG
63	AB	23	ASP
63	AB	34	MET
63	AB	37	TYR
63	AB	139	SER
64	AC	35	ASN
64	AC	46	THR
64	AC	107	GLU
64	AC	116	ASP
64	AC	117	ARG
65	AD	8	THR
65	AD	27	ASP
65	AD	72	LYS
66	AE	8	LYS
66	AE	85	ASN
66	AE	92	ASP
66	AE	104	ASP
67	AF	8	ASP
67	AF	24	LYS
67	AF	27	LYS
67	AF	33	TRP
67	AF	59	SER
68	AG	19	ARG

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Mol	Chain	Res	Type
68	AG	92	HIS
69	AH	18	SER
69	AH	22	ARG
69	AH	34	MET
69	AH	41	LYS
70	AI	9	ASP
70	AI	13	SER
70	AI	54	ASP
70	AI	87	GLU
71	AJ	19	ASP
71	AJ	97	ASN
71	AJ	105	PHE
72	AK	16	ARG
72	AK	23	MET
72	AK	47	MET
72	AK	72	PHE
72	AK	106	GLN
73	AL	50	PHE
73	AL	55	TYR
73	AL	59	CYS
73	AL	90	GLU
73	AL	101	SER
73	AL	104	ARG
74	AM	2	THR
74	AM	51	ARG
74	AM	52	ASP
74	AM	57	SER
74	AM	74	CYS
75	AN	11	SER
75	AN	17	ARG
75	AN	80	ARG
76	AO	13	ARG
76	AO	41	SER
76	AO	51	ARG
77	AP	38	MET
77	AP	48	LYS
78	AQ	88	GLN
78	AQ	99	LYS
79	AR	17	TRP
79	AR	65	PHE
79	AR	68	ASP
79	AR	194	TYR

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Mol	Chain	Res	Type
79	AR	225	LYS
79	AR	271	LYS
79	AR	286	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
12	M	206	GLN
52	0	74	GLN
53	1	209	HIS
55	3	65	GLN
55	3	110	ASN
55	3	197	GLN
57	5	146	GLN
75	AN	83	GLN
78	AQ	88	GLN
79	AR	117	ASN
79	AR	143	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	13/14 (92%)	1 (7%)	0
2	B	73/75 (97%)	13 (17%)	0
2	C	73/75 (97%)	12 (16%)	2 (2%)
3	D	3494/5070 (68%)	621 (17%)	26 (0%)
4	E	119/120 (99%)	15 (12%)	0
48	w	1618/1869 (86%)	388 (23%)	0
5	F	155/156 (99%)	28 (18%)	3 (1%)
All	All	5545/7379 (75%)	1078 (19%)	31 (0%)

All (1078) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	29	A
2	B	4	U
2	B	9	1MA
2	B	12	A
2	B	13	PSU
2	B	17	G

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Mol	Chain	Res	Type
2	B	21	A
2	B	46	A
2	B	47	5MC
2	B	48	5MC
2	B	53	5MU
2	B	73	C
2	B	74	C
2	B	75	A
2	C	4	U
2	C	6	2MG
2	C	9	1MA
2	C	17	G
2	C	18	G
2	C	21	A
2	C	26	C
2	C	46	A
2	C	47	5MC
2	C	48	5MC
2	C	53	5MU
2	C	73	C
3	D	2	G
3	D	39	A
3	D	42	A
3	D	48	G
3	D	56	A
3	D	59	A
3	D	64	A
3	D	65	A
3	D	69	A
3	D	91	G
3	D	98	A
3	D	108	A
3	D	109	G
3	D	110	C
3	D	116	G
3	D	117	C
3	D	119	G
3	D	120	A
3	D	143	C
3	D	144	G
3	D	152	U
3	D	159	C

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Mol	Chain	Res	Type
3	D	170	C
3	D	171	U
3	D	172	C
3	D	180	C
3	D	181	C
3	D	183	C
3	D	185	C
3	D	186	G
3	D	188	G
3	D	189	G
3	D	200	U
3	D	209	U
3	D	210	C
3	D	218	A
3	D	220	C
3	D	234	G
3	D	256	G
3	D	257	C
3	D	259	C
3	D	261	G
3	D	265	C
3	D	266	C
3	D	267	G
3	D	269	G
3	D	275	C
3	D	276	C
3	D	280	G
3	D	296	A
3	D	306	A
3	D	315	G
3	D	316	U
3	D	340	C
3	D	344	A
3	D	345	C
3	D	350	C
3	D	387	G
3	D	407	A
3	D	410	A
3	D	412	G
3	D	413	G
3	D	449	C
3	D	450	G

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Mol	Chain	Res	Type
3	D	452	A
3	D	453	G
3	D	454	U
3	D	467	U
3	D	468	U
3	D	484	U
3	D	485	C
3	D	486	C
3	D	487	G
3	D	491	G
3	D	494	U
3	D	495	C
3	D	496	G
3	D	498	C
3	D	499	G
3	D	500	G
3	D	507	G
3	D	509	A
3	D	510	U
3	D	513	U
3	D	514	U
3	D	515	C
3	D	516	C
3	D	517	C
3	D	645	G
3	D	657	C
3	D	659	G
3	D	661	C
3	D	665	C
3	D	667	A
3	D	668	C
3	D	670	G
3	D	673	C
3	D	686	A
3	D	688	U
3	D	703	G
3	D	704	C
3	D	731	G
3	D	738	C
3	D	739	G
3	D	740	G
3	D	746	A

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Mol	Chain	Res	Type
3	D	754	U
3	D	760	G
3	D	904	C
3	D	905	C
3	D	913	U
3	D	914	U
3	D	915	A
3	D	917	A
3	D	918	G
3	D	923	C
3	D	924	C
3	D	926	G
3	D	932	A
3	D	933	G
3	D	935	A
3	D	936	C
3	D	937	U
3	D	943	A
3	D	944	A
3	D	945	U
3	D	959	G
3	D	960	A
3	D	961	G
3	D	962	C
3	D	965	G
3	D	966	A
3	D	970	G
3	D	971	U
3	D	972	C
3	D	977	C
3	D	982	U
3	D	984	C
3	D	988	C
3	D	989	U
3	D	1071	C
3	D	1075	G
3	D	1082	C
3	D	1083	U
3	D	1094	G
3	D	1168	G
3	D	1170	G
3	D	1171	G

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Mol	Chain	Res	Type
3	D	1173	G
3	D	1178	G
3	D	1179	U
3	D	1180	C
3	D	1181	C
3	D	1182	C
3	D	1183	C
3	D	1184	A
3	D	1192	C
3	D	1193	C
3	D	1196	G
3	D	1202	C
3	D	1203	G
3	D	1211	G
3	D	1214	C
3	D	1215	C
3	D	1217	G
3	D	1219	G
3	D	1241	C
3	D	1262	G
3	D	1266	G
3	D	1269	G
3	D	1270	A
3	D	1271	G
3	D	1272	C
3	D	1273	G
3	D	1275	G
3	D	1277	G
3	D	1280	C
3	D	1284	G
3	D	1285	U
3	D	1287	G
3	D	1294	A
3	D	1295	C
3	D	1296	G
3	D	1301	C
3	D	1302	U
3	D	1303	A
3	D	1304	C
3	D	1313	C
3	D	1326	A2M
3	D	1337	A

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Mol	Chain	Res	Type
3	D	1354	A
3	D	1358	G
3	D	1359	G
3	D	1365	C
3	D	1366	G
3	D	1377	G
3	D	1379	C
3	D	1387	A
3	D	1393	G
3	D	1394	G
3	D	1397	A
3	D	1398	A
3	D	1403	G
3	D	1404	G
3	D	1407	C
3	D	1408	G
3	D	1409	C
3	D	1410	U
3	D	1411	C
3	D	1412	G
3	D	1415	G
3	D	1417	C
3	D	1420	A
3	D	1439	C
3	D	1442	C
3	D	1443	A
3	D	1452	A
3	D	1481	C
3	D	1482	G
3	D	1483	C
3	D	1497	A
3	D	1498	G
3	D	1502	G
3	D	1514	U
3	D	1534	A2M
3	D	1547	A
3	D	1564	A
3	D	1566	C
3	D	1575	A
3	D	1578	U
3	D	1591	U
3	D	1596	U

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Mol	Chain	Res	Type
3	D	1624	G
3	D	1625	OMG
3	D	1631	A
3	D	1633	G
3	D	1634	A
3	D	1640	C
3	D	1641	G
3	D	1642	A
3	D	1654	G
3	D	1661	C
3	D	1676	C
3	D	1677	PSU
3	D	1678	C
3	D	1698	C
3	D	1699	A
3	D	1700	G
3	D	1701	A
3	D	1702	C
3	D	1703	C
3	D	1705	G
3	D	1715	C
3	D	1716	G
3	D	1734	G
3	D	1735	U
3	D	1741	G
3	D	1742	A
3	D	1750	G
3	D	1756	U
3	D	1757	U
3	D	1758	G
3	D	1760	OMG
3	D	1763	C
3	D	1787	A
3	D	1797	G
3	D	1804	A
3	D	1810	G
3	D	1821	G
3	D	1822	U
3	D	1834	U
3	D	1836	G
3	D	1837	A
3	D	1842	G

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Mol	Chain	Res	Type
3	D	1843	A
3	D	1855	G
3	D	1869	G
3	D	1882	U
3	D	1889	U
3	D	1897	A
3	D	1918	U
3	D	1919	G
3	D	1920	C
3	D	1921	C
3	D	1922	G
3	D	1925	G
3	D	1931	C
3	D	1932	A
3	D	1940	G
3	D	1948	G
3	D	1951	G
3	D	1959	U
3	D	1960	A
3	D	1961	G
3	D	1962	A
3	D	2024	G
3	D	2025	A
3	D	2026	A
3	D	2046	G
3	D	2048	U
3	D	2055	G
3	D	2056	G
3	D	2069	A
3	D	2084	C
3	D	2085	G
3	D	2089	G
3	D	2092	G
3	D	2093	A
3	D	2095	A
3	D	2096	G
3	D	2097	U
3	D	2098	G
3	D	2099	G
3	D	2102	G
3	D	2103	G
3	D	2104	G

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Mol	Chain	Res	Type
3	D	2105	A
3	D	2107	C
3	D	2257	C
3	D	2258	C
3	D	2259	G
3	D	2289	C
3	D	2300	A
3	D	2301	G
3	D	2313	A
3	D	2316	G
3	D	2333	G
3	D	2348	G
3	D	2351	OMC
3	D	2395	A
3	D	2397	G
3	D	2415	OMU
3	D	2416	G
3	D	2421	G
3	D	2422	OMC
3	D	2424	OMG
3	D	2425	U
3	D	2450	G
3	D	2453	A
3	D	2465	C
3	D	2474	G
3	D	2475	G
3	D	2479	G
3	D	2483	G
3	D	2484	A
3	D	2485	U
3	D	2487	G
3	D	2488	C
3	D	2489	C
3	D	2491	C
3	D	2493	G
3	D	2494	U
3	D	2503	G
3	D	2504	C
3	D	2505	C
3	D	2506	G
3	D	2511	A
3	D	2513	A

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Mol	Chain	Res	Type
3	D	2519	U
3	D	2520	C
3	D	2529	A
3	D	2537	A
3	D	2545	U
3	D	2546	G
3	D	2547	G
3	D	2554	U
3	D	2567	G
3	D	2583	C
3	D	2587	A
3	D	2601	A
3	D	2618	G
3	D	2627	C
3	D	2653	C
3	D	2662	G
3	D	2669	C
3	D	2676	A
3	D	2687	U
3	D	2694	G
3	D	2695	A
3	D	2696	A
3	D	2706	G
3	D	2707	U
3	D	2708	U
3	D	2711	G
3	D	2712	G
3	D	2721	G
3	D	2724	G
3	D	2726	G
3	D	2739	C
3	D	2742	G
3	D	2743	A
3	D	2746	A
3	D	2754	G
3	D	2760	G
3	D	2761	U
3	D	2763	U
3	D	2764	A
3	D	2770	C
3	D	2788	U
3	D	2790	U

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Mol	Chain	Res	Type
3	D	2814	C
3	D	2815	A2M
3	D	2826	U
3	D	2827	G
3	D	2838	G
3	D	2855	G
3	D	2856	C
3	D	2867	C
3	D	2874	U
3	D	2877	G
3	D	2892	C
3	D	2900	U
3	D	3604	A
3	D	3605	C
3	D	3615	G
3	D	3618	C
3	D	3626	G
3	D	3635	A
3	D	3644	U
3	D	3648	A
3	D	3662	A
3	D	3664	G
3	D	3673	C
3	D	3674	G
3	D	3711	A
3	D	3712	A
3	D	3735	G
3	D	3736	A
3	D	3748	A
3	D	3750	G
3	D	3753	G
3	D	3757	G
3	D	3758	PSU
3	D	3760	A2M
3	D	3763	A
3	D	3771	C
3	D	3776	G
3	D	3777	G
3	D	3783	A
3	D	3784	A
3	D	3786	U
3	D	3802	U

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Mol	Chain	Res	Type
3	D	3811	G
3	D	3812	C
3	D	3814	U
3	D	3817	A
3	D	3819	G
3	D	3823	G
3	D	3838	U
3	D	3840	U
3	D	3867	A
3	D	3877	A
3	D	3878	C
3	D	3879	G
3	D	3885	G
3	D	3897	G
3	D	3901	A
3	D	3906	A
3	D	3907	G
3	D	3908	A
3	D	3915	U
3	D	3938	G
3	D	3939	G
3	D	3943	A
3	D	3944	OMG
3	D	3946	G
3	D	4076	G
3	D	4086	G
3	D	4093	G
3	D	4094	G
3	D	4097	G
3	D	4098	A
3	D	4113	U
3	D	4114	C
3	D	4115	G
3	D	4116	C
3	D	4119	C
3	D	4122	G
3	D	4127	A
3	D	4140	C
3	D	4142	C
3	D	4143	G
3	D	4144	C
3	D	4145	C

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Mol	Chain	Res	Type
3	D	4150	G
3	D	4162	C
3	D	4163	U
3	D	4170	A
3	D	4183	G
3	D	4184	G
3	D	4191	G
3	D	4203	A
3	D	4229	U
3	D	4233	A
3	D	4251	A
3	D	4254	G
3	D	4257	A
3	D	4268	A
3	D	4273	A
3	D	4281	A
3	D	4291	G
3	D	4297	G
3	D	4304	A
3	D	4305	G
3	D	4314	C
3	D	4330	G
3	D	4332	C
3	D	4339	A
3	D	4349	C
3	D	4364	G
3	D	4373	G
3	D	4376	A
3	D	4377	G
3	D	4378	A
3	D	4380	A
3	D	4387	C
3	D	4391	G
3	D	4394	A
3	D	4405	G
3	D	4421	C
3	D	4422	A
3	D	4444	C
3	D	4448	G
3	D	4449	A
3	D	4452	U
3	D	4453	C

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Mol	Chain	Res	Type
3	D	4464	A
3	D	4466	C
3	D	4475	G
3	D	4500	PSU
3	D	4512	U
3	D	4513	A
3	D	4519	C
3	D	4524	G
3	D	4545	G
3	D	4548	A
3	D	4554	G
3	D	4560	C
3	D	4567	G
3	D	4570	G
3	D	4573	G
3	D	4575	G
3	D	4590	A
3	D	4600	G
3	D	4601	U
3	D	4617	G
3	D	4636	U
3	D	4637	OMG
3	D	4656	A
3	D	4670	C
3	D	4672	A
3	D	4679	G
3	D	4695	C
3	D	4700	A
3	D	4708	A
3	D	4709	U
3	D	4719	G
3	D	4720	C
3	D	4730	C
3	D	4731	G
3	D	4732	G
3	D	4733	C
3	D	4734	A
3	D	4741	C
3	D	4742	G
3	D	4745	G
3	D	4754	G
3	D	4757	C

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Mol	Chain	Res	Type
3	D	4759	C
3	D	4761	G
3	D	4765	G
3	D	4774	C
3	D	4860	G
3	D	4862	G
3	D	4870	G
3	D	4871	C
3	D	4875	G
3	D	4882	U
3	D	4883	C
3	D	4888	U
3	D	4889	G
3	D	4895	C
3	D	4896	G
3	D	4899	G
3	D	4900	C
3	D	4901	G
3	D	4902	C
3	D	4910	G
3	D	4912	G
3	D	4914	C
3	D	4927	G
3	D	4928	C
3	D	4934	A
3	D	4940	C
3	D	4941	G
3	D	4943	A
3	D	4955	A
3	D	4960	G
3	D	4963	G
3	D	4966	A
3	D	4976	U
3	D	4985	U
3	D	4989	U
3	D	4990	C
3	D	4991	U
3	D	5014	A
3	D	5016	A
3	D	5017	G
3	D	5024	C
3	D	5025	C

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Mol	Chain	Res	Type
3	D	5026	U
3	D	5028	G
3	D	5030	U
3	D	5034	A
3	D	5041	G
3	D	5050	C
3	D	5054	C
3	D	5060	A
3	D	5061	A
3	D	5062	G
3	D	5069	U
4	E	7	G
4	E	22	A
4	E	31	G
4	E	47	G
4	E	48	G
4	E	53	U
4	E	54	A
4	E	64	G
4	E	97	G
4	E	100	A
4	E	102	U
4	E	103	A
4	E	110	G
4	E	117	G
4	E	120	U
5	F	2	G
5	F	17	A
5	F	23	C
5	F	34	U
5	F	35	C
5	F	48	A
5	F	59	A
5	F	63	U
5	F	80	A
5	F	81	C
5	F	82	A
5	F	83	C
5	F	84	A
5	F	85	U
5	F	86	U
5	F	87	G

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Mol	Chain	Res	Type
5	F	103	A
5	F	105	C
5	F	110	U
5	F	114	G
5	F	124	U
5	F	125	C
5	F	126	C
5	F	127	U
5	F	128	C
5	F	150	C
5	F	151	G
5	F	153	C
48	w	2	A
48	w	17	C
48	w	21	U
48	w	22	A
48	w	33	G
48	w	34	PSU
48	w	35	C
48	w	41	G
48	w	43	U
48	w	44	U
48	w	45	A
48	w	46	A
48	w	49	C
48	w	59	U
48	w	60	A
48	w	61	A
48	w	62	G
48	w	66	G
48	w	67	C
48	w	68	A
48	w	69	C
48	w	78	C
48	w	79	A
48	w	80	G
48	w	81	U
48	w	83	A
48	w	89	C
48	w	97	U
48	w	103	A
48	w	112	U

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Mol	Chain	Res	Type
48	w	113	G
48	w	115	U
48	w	116	OMU
48	w	120	U
48	w	121	OMU
48	w	126	G
48	w	129	C
48	w	130	G
48	w	143	U
48	w	149	A
48	w	150	A
48	w	154	U
48	w	155	G
48	w	159	A2M
48	w	161	U
48	w	162	C
48	w	163	U
48	w	166	A2M
48	w	173	A
48	w	182	C
48	w	190	G
48	w	191	A
48	w	194	C
48	w	195	C
48	w	196	C
48	w	197	U
48	w	198	U
48	w	199	C
48	w	200	G
48	w	214	U
48	w	215	G
48	w	226	A
48	w	291	G
48	w	292	A
48	w	293	C
48	w	294	U
48	w	295	C
48	w	311	C
48	w	312	G
48	w	313	A
48	w	318	A
48	w	319	C

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Mol	Chain	Res	Type
48	w	332	G
48	w	345	U
48	w	346	C
48	w	347	G
48	w	362	C
48	w	364	A
48	w	370	G
48	w	380	G
48	w	381	C
48	w	385	G
48	w	386	C
48	w	398	A
48	w	400	C
48	w	407	G
48	w	408	A
48	w	409	C
48	w	413	G
48	w	418	A
48	w	421	G
48	w	428	OMU
48	w	438	G
48	w	441	C
48	w	447	A
48	w	448	A
48	w	449	A
48	w	450	C
48	w	451	G
48	w	452	G
48	w	464	A
48	w	466	G
48	w	467	G
48	w	468	A2M
48	w	471	G
48	w	472	C
48	w	473	A
48	w	474	G
48	w	482	G
48	w	485	A
48	w	487	U
48	w	488	U
48	w	489	A
48	w	491	C

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Mol	Chain	Res	Type
48	w	493	A
48	w	496	C
48	w	497	C
48	w	498	C
48	w	500	A
48	w	506	G
48	w	507	G
48	w	512	A2M
48	w	516	A
48	w	519	A
48	w	523	A
48	w	528	A
48	w	531	A
48	w	532	C
48	w	533	A
48	w	534	G
48	w	551	U
48	w	552	G
48	w	554	A
48	w	556	U
48	w	557	U
48	w	558	G
48	w	560	A
48	w	575	A
48	w	576	A2M
48	w	583	C
48	w	587	A
48	w	588	G
48	w	589	G
48	w	590	A2M
48	w	592	C
48	w	594	A
48	w	595	U
48	w	596	U
48	w	597	G
48	w	598	G
48	w	604	A
48	w	605	A
48	w	606	G
48	w	608	C
48	w	614	C
48	w	616	A

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Mol	Chain	Res	Type
48	w	617	G
48	w	627	OMU
48	w	628	A
48	w	632	C
48	w	643	A
48	w	655	A
48	w	659	G
48	w	660	C
48	w	664	A
48	w	668	A2M
48	w	669	A
48	w	671	A
48	w	672	A
48	w	688	U
48	w	810	A
48	w	811	A
48	w	812	A
48	w	821	G
48	w	822	PSU
48	w	830	A
48	w	834	C
48	w	835	C
48	w	836	G
48	w	837	A
48	w	838	G
48	w	839	C
48	w	840	C
48	w	841	G
48	w	842	C
48	w	847	A
48	w	853	C
48	w	869	A
48	w	870	A
48	w	872	A
48	w	874	G
48	w	878	G
48	w	880	G
48	w	881	G
48	w	882	U
48	w	883	U
48	w	884	C
48	w	888	U

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Mol	Chain	Res	Type
48	w	889	U
48	w	890	U
48	w	891	G
48	w	893	U
48	w	895	G
48	w	896	U
48	w	897	U
48	w	898	U
48	w	899	U
48	w	900	C
48	w	901	G
48	w	904	A
48	w	909	G
48	w	912	C
48	w	913	A
48	w	917	U
48	w	920	A
48	w	930	C
48	w	933	G
48	w	934	G
48	w	943	U
48	w	958	G
48	w	963	A
48	w	970	G
48	w	990	A
48	w	992	A
48	w	999	G
48	w	1001	A
48	w	1017	U
48	w	1023	A
48	w	1027	A
48	w	1032	C
48	w	1060	A
48	w	1061	U
48	w	1062	A
48	w	1083	A
48	w	1085	C
48	w	1109	C
48	w	1114	U
48	w	1115	U
48	w	1116	C
48	w	1118	C

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Mol	Chain	Res	Type
48	w	1119	A
48	w	1126	G
48	w	1133	A
48	w	1153	C
48	w	1154	U
48	w	1157	G
48	w	1183	A
48	w	1195	A
48	w	1207	G
48	w	1208	A
48	w	1215	C
48	w	1217	A
48	w	1221	G
48	w	1224	G
48	w	1242	U
48	w	1243	U
48	w	1251	A
48	w	1253	A
48	w	1256	G
48	w	1257	G
48	w	1259	A
48	w	1265	A
48	w	1271	C
48	w	1274	G
48	w	1275	G
48	w	1284	A
48	w	1285	G
48	w	1288	OMU
48	w	1293	A
48	w	1295	A
48	w	1298	G
48	w	1301	A
48	w	1302	G
48	w	1308	U
48	w	1309	C
48	w	1332	A
48	w	1342	U
48	w	1371	U
48	w	1372	U
48	w	1373	C
48	w	1378	A
48	w	1396	A

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Mol	Chain	Res	Type
48	w	1397	U
48	w	1401	A
48	w	1402	A
48	w	1403	C
48	w	1404	U
48	w	1408	U
48	w	1417	C
48	w	1428	G
48	w	1429	G
48	w	1430	C
48	w	1433	C
48	w	1434	C
48	w	1435	C
48	w	1436	C
48	w	1438	A
48	w	1447	G
48	w	1449	G
48	w	1450	G
48	w	1452	A
48	w	1454	A
48	w	1462	U
48	w	1463	U
48	w	1464	C
48	w	1476	A
48	w	1477	U
48	w	1487	A
48	w	1489	A
48	w	1490	OMG
48	w	1495	G
48	w	1497	G
48	w	1498	A
48	w	1508	A
48	w	1515	G
48	w	1521	C
48	w	1522	A
48	w	1523	C
48	w	1528	G
48	w	1533	A
48	w	1536	G
48	w	1543	U
48	w	1545	A
48	w	1546	G

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Mol	Chain	Res	Type
48	w	1548	G
48	w	1550	G
48	w	1551	U
48	w	1552	G
48	w	1553	C
48	w	1555	U
48	w	1556	A
48	w	1569	A
48	w	1570	G
48	w	1574	C
48	w	1580	A
48	w	1585	U
48	w	1586	U
48	w	1588	A
48	w	1599	U
48	w	1601	A
48	w	1602	U
48	w	1607	A
48	w	1610	G
48	w	1621	U
48	w	1623	A
48	w	1624	U
48	w	1630	A
48	w	1632	G
48	w	1633	A
48	w	1635	C
48	w	1637	A
48	w	1639	G7M
48	w	1640	A
48	w	1648	G
48	w	1654	G
48	w	1663	A
48	w	1665	G
48	w	1671	G
48	w	1680	G
48	w	1698	C
48	w	1721	U
48	w	1722	G
48	w	1742	C
48	w	1744	G
48	w	1745	A
48	w	1748	G

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Mol	Chain	Res	Type
48	w	1751	C
48	w	1753	C
48	w	1754	G
48	w	1778	C
48	w	1779	G
48	w	1782	G
48	w	1783	C
48	w	1784	G
48	w	1786	U
48	w	1801	A
48	w	1813	A
48	w	1824	A
48	w	1829	G
48	w	1831	A
48	w	1838	U
48	w	1849	G
48	w	1852	C
48	w	1861	G
48	w	1862	G
48	w	1863	A
48	w	1865	C
48	w	1869	A

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	5	C
2	C	72	G
3	D	1	C
3	D	406	C
3	D	515	C
3	D	914	U
3	D	922	C
3	D	987	C
3	D	1081	C
3	D	1574	G
3	D	1625	OMG
3	D	1633	G
3	D	1755	C
3	D	2101	C
3	D	2102	G
3	D	2675	G

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Mol	Chain	Res	Type
3	D	3614	G
3	D	3673	C
3	D	4092	G
3	D	4113	U
3	D	4115	G
3	D	4348	A
3	D	4378	A
3	D	4600	G
3	D	4678	G
3	D	4699	U
3	D	4913	G
3	D	5016	A
5	F	16	G
5	F	86	U
5	F	126	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5MC	B	47	2	18,22,23	3.75	8 (44%)	26,32,35	1.05	2 (7%)
48	A2M	w	668	48,80	18,25,26	1.58	2 (11%)	18,36,39	0.95	1 (5%)
48	PSU	w	1625	48	18,21,22	1.07	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	1677	3	18,21,22	1.06	2 (11%)	22,30,33	1.75	4 (18%)
2	5MU	B	53	2	19,22,23	4.66	5 (26%)	28,32,35	3.64	8 (28%)
3	PSU	D	3762	3	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
3	6MZ	D	4220	3	18,25,26	2.01	2 (11%)	16,36,39	2.08	3 (18%)
3	OMC	D	2351	80,3	19,22,23	2.80	7 (36%)	26,31,34	0.77	0
48	PSU	w	119	48	18,21,22	1.06	1 (5%)	22,30,33	1.76	4 (18%)
3	UY1	D	3818	80,3	19,22,23	1.10	2 (10%)	22,31,34	0.92	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	2MG	C	6	2	18,26,27	2.20	5 (27%)	16,38,41	1.44	3 (18%)
3	PSU	D	4972	80,3	18,21,22	1.02	1 (5%)	22,30,33	1.85	4 (18%)
3	PSU	D	4500	2,3	18,21,22	1.10	1 (5%)	22,30,33	1.84	4 (18%)
48	PSU	w	966	48	18,21,22	1.03	1 (5%)	22,30,33	1.82	5 (22%)
48	OMU	w	116	48	19,22,23	2.92	8 (42%)	26,31,34	1.70	4 (15%)
48	4AC	w	1842	48	21,24,25	0.56	0	29,34,37	1.16	4 (13%)
48	A2M	w	27	48	18,25,26	1.50	1 (5%)	18,36,39	0.98	0
48	PSU	w	1347	48	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	D	4552	3	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
2	5MC	C	48	2	18,22,23	3.79	8 (44%)	26,32,35	1.02	2 (7%)
3	PSU	D	3770	3	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4420	3	18,21,22	1.04	1 (5%)	22,30,33	1.80	5 (22%)
3	OMG	D	4228	3	18,26,27	2.73	8 (44%)	19,38,41	1.57	4 (21%)
3	PSU	D	4521	80,3	18,21,22	1.04	1 (5%)	22,30,33	1.88	5 (22%)
48	PSU	w	686	48	18,21,22	1.05	1 (5%)	22,30,33	1.82	4 (18%)
48	PSU	w	406	48	18,21,22	1.03	1 (5%)	22,30,33	1.86	5 (22%)
3	OMG	D	3944	3	18,26,27	2.81	8 (44%)	19,38,41	1.50	4 (21%)
48	B8N	w	1248	48	24,29,30	0.80	0	29,42,45	0.97	2 (6%)
3	A2M	D	3825	3	18,25,26	1.49	1 (5%)	18,36,39	1.04	1 (5%)
3	A2M	D	1326	3	18,25,26	1.45	1 (5%)	18,36,39	1.03	1 (5%)
3	PSU	D	5001	80,3	18,21,22	1.03	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	1860	3	18,21,22	1.05	1 (5%)	22,30,33	1.86	4 (18%)
48	A2M	w	99	48,80	18,25,26	1.47	1 (5%)	18,36,39	1.02	1 (5%)
48	OMG	w	1490	48,80	18,26,27	2.76	8 (44%)	19,38,41	1.47	4 (21%)
3	OMU	D	2837	3	19,22,23	2.75	6 (31%)	26,31,34	1.85	5 (19%)
48	MA6	w	1850	48	19,26,27	1.03	1 (5%)	18,38,41	1.60	3 (16%)
3	OMC	D	4456	3	19,22,23	2.82	8 (42%)	26,31,34	0.69	0
2	H2U	C	19	2	18,21,22	1.06	2 (11%)	21,30,33	0.80	0
48	PSU	w	1045	48	18,21,22	1.04	1 (5%)	22,30,33	1.87	5 (22%)
2	1MA	C	9	2	16,25,26	0.96	1 (6%)	18,37,40	0.82	0
48	PSU	w	93	48	18,21,22	1.05	1 (5%)	22,30,33	1.78	3 (13%)
3	PSU	D	3764	3	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	OMC	D	2824	3	19,22,23	2.86	8 (42%)	26,31,34	0.72	0
3	PSU	D	4442	3	18,21,22	1.05	1 (5%)	22,30,33	1.86	6 (27%)
3	PSU	D	3851	3	18,21,22	1.03	1 (5%)	22,30,33	1.87	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
3	OMU	D	2415	3	19,22,23	2.83	6 (31%)	26,31,34	1.94	6 (23%)
3	PSU	D	2508	3	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	D	4293	3	18,21,22	1.06	2 (11%)	22,30,33	1.83	4 (18%)
3	OMG	D	4499	2,3	18,26,27	2.74	8 (44%)	19,38,41	1.50	4 (21%)
48	PSU	w	1004	48	18,21,22	1.06	1 (5%)	22,30,33	1.82	4 (18%)
48	4AC	w	1337	48	21,24,25	0.56	0	29,34,37	1.19	5 (17%)
3	PSU	D	3730	3	18,21,22	1.02	1 (5%)	22,30,33	1.82	5 (22%)
48	PSU	w	815	48	18,21,22	1.08	1 (5%)	22,30,33	1.86	5 (22%)
48	PSU	w	1643	48,80	18,21,22	1.04	1 (5%)	22,30,33	1.81	5 (22%)
2	5MC	C	47	2	18,22,23	3.79	8 (44%)	26,32,35	1.04	2 (7%)
3	1MA	D	1322	3	16,25,26	0.87	0	18,37,40	0.88	0
3	OMG	D	4637	3	18,26,27	2.73	8 (44%)	19,38,41	1.50	4 (21%)
48	OMU	w	1326	48	19,22,23	2.88	7 (36%)	26,31,34	1.78	6 (23%)
2	H2U	B	19	2	18,21,22	1.09	2 (11%)	21,30,33	0.82	0
3	OMU	D	1773	3	19,22,23	2.92	8 (42%)	26,31,34	1.68	4 (15%)
3	OMU	D	4498	80,3	19,22,23	2.79	6 (31%)	26,31,34	1.75	5 (19%)
2	5MU	C	53	2	19,22,23	4.66	6 (31%)	28,32,35	3.61	9 (32%)
3	OMG	D	1316	3	18,26,27	2.73	8 (44%)	19,38,41	1.55	4 (21%)
3	OMG	D	1522	3	18,26,27	2.68	8 (44%)	19,38,41	1.50	4 (21%)
3	PSU	D	3920	80,3	18,21,22	1.02	1 (5%)	22,30,33	1.85	4 (18%)
48	OMG	w	644	48	18,26,27	2.83	8 (44%)	19,38,41	1.50	4 (21%)
48	OMC	w	1703	48,80	19,22,23	2.89	8 (42%)	26,31,34	0.73	0
3	OMU	D	3925	3	19,22,23	2.78	6 (31%)	26,31,34	1.84	5 (19%)
3	PSU	D	4576	3	18,21,22	1.02	1 (5%)	22,30,33	1.84	4 (18%)
48	PSU	w	1367	48	18,21,22	1.04	1 (5%)	22,30,33	1.87	5 (22%)
3	OMU	D	4227	3	19,22,23	2.81	6 (31%)	26,31,34	1.75	4 (15%)
2	5MC	B	48	2	18,22,23	3.79	8 (44%)	26,32,35	1.03	2 (7%)
2	1MA	C	57	2	16,25,26	0.94	1 (6%)	18,37,40	0.85	0
3	A2M	D	1524	3	18,25,26	1.59	2 (11%)	18,36,39	1.00	1 (5%)
3	OMG	D	4494	3	18,26,27	2.75	8 (44%)	19,38,41	1.51	4 (21%)
48	PSU	w	822	48	18,21,22	1.08	1 (5%)	22,30,33	1.75	5 (22%)
48	PSU	w	1056	48	18,21,22	1.02	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	1792	3	18,21,22	0.99	1 (5%)	22,30,33	1.76	3 (13%)
3	OMC	D	2422	80,3	19,22,23	2.87	8 (42%)	26,31,34	0.73	0
2	2MG	B	6	2	18,26,27	2.19	5 (27%)	16,38,41	1.47	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	PSU	w	218	48	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
48	OMG	w	436	48	18,26,27	2.82	8 (44%)	19,38,41	1.55	4 (21%)
3	PSU	D	4423	3	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	3758	3	18,21,22	0.97	1 (5%)	22,30,33	1.81	4 (18%)
2	5MC	C	38	2	18,22,23	3.76	8 (44%)	26,32,35	1.02	2 (7%)
48	PSU	w	681	48,80	18,21,22	1.04	1 (5%)	22,30,33	1.90	5 (22%)
3	A2M	D	3785	80,3	18,25,26	1.55	2 (11%)	18,36,39	1.23	1 (5%)
3	OMG	D	4370	3	18,26,27	2.73	8 (44%)	19,38,41	1.50	4 (21%)
3	A2M	D	400	3	18,25,26	1.52	1 (5%)	18,36,39	1.03	1 (5%)
3	5MC	D	4447	80,3	18,22,23	3.60	7 (38%)	26,32,35	1.13	1 (3%)
2	56B	B	34	2	27,35,36	3.03	13 (48%)	28,52,55	4.60	4 (14%)
3	OMC	D	2861	3	19,22,23	2.85	8 (42%)	26,31,34	0.67	0
48	OMG	w	601	48	18,26,27	2.82	8 (44%)	19,38,41	1.50	4 (21%)
3	PSU	D	3715	3	18,21,22	1.05	1 (5%)	22,30,33	1.85	5 (22%)
48	PSU	w	651	48	18,21,22	1.03	1 (5%)	22,30,33	1.87	5 (22%)
3	PSU	D	3695	3	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
48	PSU	w	105	48	18,21,22	1.04	1 (5%)	22,30,33	1.81	5 (22%)
48	A2M	w	512	48	18,25,26	1.50	1 (5%)	18,36,39	1.08	1 (5%)
48	OMU	w	1288	48	19,22,23	2.96	8 (42%)	26,31,34	1.67	4 (15%)
48	OMU	w	1442	48,80	19,22,23	2.87	6 (31%)	26,31,34	1.70	5 (19%)
48	PSU	w	1445	48	18,21,22	1.04	1 (5%)	22,30,33	1.81	5 (22%)
3	PSU	D	1536	3	18,21,22	1.05	2 (11%)	22,30,33	1.88	4 (18%)
3	PSU	D	4457	3	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
48	6MZ	w	1832	48,80	18,25,26	1.99	3 (16%)	16,36,39	1.87	2 (12%)
3	PSU	D	4471	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	4431	3	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
48	PSU	w	801	48	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	4579	3	18,21,22	1.04	1 (5%)	22,30,33	1.83	4 (18%)
3	OMU	D	4620	3	19,22,23	2.76	6 (31%)	26,31,34	1.78	5 (19%)
2	5MC	B	38	2	18,22,23	3.71	8 (44%)	26,32,35	1.06	2 (7%)
3	OMC	D	3701	80,3	19,22,23	2.85	8 (42%)	26,31,34	0.73	0
48	OMC	w	462	48	19,22,23	3.01	8 (42%)	26,31,34	0.74	0
3	A2M	D	3760	3	18,25,26	1.46	1 (5%)	18,36,39	1.25	2 (11%)
48	PSU	w	863	48	18,21,22	1.08	1 (5%)	22,30,33	1.82	5 (22%)
48	PSU	w	572	48	18,21,22	1.09	1 (5%)	22,30,33	1.79	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	PSU	C	13	2	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
48	OMG	w	1328	48	18,26,27	2.82	8 (44%)	19,38,41	1.49	4 (21%)
48	A2M	w	468	48	18,25,26	1.59	1 (5%)	18,36,39	1.02	0
2	1MA	B	9	2	16,25,26	0.93	1 (6%)	18,37,40	0.86	0
5	OMG	F	75	5	18,26,27	2.77	8 (44%)	19,38,41	1.49	4 (21%)
48	OMU	w	428	48	19,22,23	2.93	8 (42%)	26,31,34	1.71	5 (19%)
3	PSU	D	3639	3	18,21,22	1.04	1 (5%)	22,30,33	1.76	4 (18%)
48	A2M	w	484	48	18,25,26	1.55	1 (5%)	18,36,39	1.03	1 (5%)
3	PSU	D	4299	3	18,21,22	1.03	1 (5%)	22,30,33	1.84	4 (18%)
3	A2M	D	398	3	18,25,26	1.46	1 (5%)	18,36,39	1.01	1 (5%)
2	56B	C	34	2	27,35,36	3.02	12 (44%)	28,52,55	4.67	4 (14%)
48	A2M	w	1678	48	18,25,26	1.50	1 (5%)	18,36,39	0.99	1 (5%)
48	OMU	w	1804	48	19,22,23	2.86	6 (31%)	26,31,34	1.76	4 (15%)
3	OMC	D	3808	3	19,22,23	2.84	8 (42%)	26,31,34	0.76	0
3	PSU	D	1862	3	18,21,22	1.03	1 (5%)	22,30,33	1.89	5 (22%)
48	OMU	w	121	48	19,22,23	2.94	8 (42%)	26,31,34	1.65	4 (15%)
48	A2M	w	159	48	18,25,26	1.57	1 (5%)	18,36,39	1.07	1 (5%)
2	PSU	B	13	2	18,21,22	1.03	1 (5%)	22,30,33	1.86	5 (22%)
3	PSU	D	4296	3	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	D	4353	3	18,21,22	1.03	1 (5%)	22,30,33	1.85	4 (18%)
48	OMC	w	517	48,80	19,22,23	2.99	8 (42%)	26,31,34	0.76	0
3	PSU	D	1782	3	18,21,22	1.00	1 (5%)	22,30,33	1.84	4 (18%)
3	OMG	D	3744	3	18,26,27	2.76	8 (44%)	19,38,41	1.52	4 (21%)
3	PSU	D	1683	3	18,21,22	1.07	2 (11%)	22,30,33	1.95	5 (22%)
3	OMC	D	2365	80,3	19,22,23	2.84	8 (42%)	26,31,34	0.71	0
48	OMU	w	627	48	19,22,23	2.90	7 (36%)	26,31,34	1.72	5 (19%)
48	A2M	w	166	48	18,25,26	1.50	1 (5%)	18,36,39	1.09	1 (5%)
48	OMU	w	799	48	19,22,23	2.94	8 (42%)	26,31,34	1.68	4 (15%)
3	OMG	D	1760	3	18,26,27	2.83	8 (44%)	19,38,41	1.46	4 (21%)
48	PSU	w	1232	48	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
3	A2M	D	2815	3	18,25,26	1.55	1 (5%)	18,36,39	1.00	1 (5%)
2	PSU	C	54	2	18,21,22	1.08	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	D	3792	3	18,26,27	2.70	8 (44%)	19,38,41	1.47	4 (21%)
48	PSU	w	1046	48	18,21,22	1.04	1 (5%)	22,30,33	1.83	4 (18%)
48	G7M	w	1639	48,2	20,26,27	2.71	7 (35%)	17,39,42	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	PSU	D	4403	80,3	18,21,22	1.06	1 (5%)	22,30,33	1.88	5 (22%)
48	PSU	w	1081	48	18,21,22	1.01	1 (5%)	22,30,33	1.81	4 (18%)
3	PSU	D	5010	3	18,21,22	1.03	1 (5%)	22,30,33	1.87	5 (22%)
3	PSU	D	2632	3	18,21,22	1.02	1 (5%)	22,30,33	1.80	4 (18%)
48	A2M	w	576	48	18,25,26	1.43	1 (5%)	18,36,39	1.04	1 (5%)
3	A2M	D	3718	3	18,25,26	1.48	1 (5%)	18,36,39	1.02	1 (5%)
48	PSU	w	34	48	18,21,22	1.06	1 (5%)	22,30,33	1.69	4 (18%)
3	PSU	D	3853	80,3	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
48	PSU	w	814	48	18,21,22	1.05	1 (5%)	22,30,33	1.80	4 (18%)
3	A2M	D	4523	80,3	18,25,26	1.59	2 (11%)	18,36,39	1.12	2 (11%)
3	OMC	D	4536	3	19,22,23	2.83	8 (42%)	26,31,34	0.74	0
3	PSU	D	4689	3	18,21,22	1.04	1 (5%)	22,30,33	1.81	4 (18%)
3	OMU	D	4306	3	19,22,23	2.76	6 (31%)	26,31,34	1.78	5 (19%)
3	OMG	D	4392	3	18,26,27	2.71	8 (44%)	19,38,41	1.52	4 (21%)
3	PSU	D	1744	80,3	18,21,22	1.02	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	D	4196	80,2,3	18,26,27	2.69	8 (44%)	19,38,41	1.45	4 (21%)
3	A2M	D	2363	80,3	18,25,26	1.47	2 (11%)	18,36,39	1.02	1 (5%)
3	PSU	D	3734	3	18,21,22	1.05	1 (5%)	22,30,33	1.86	5 (22%)
2	PSU	B	54	2	18,21,22	1.04	1 (5%)	22,30,33	1.76	4 (18%)
48	OMC	w	174	48	19,22,23	3.02	8 (42%)	26,31,34	0.77	0
3	OMG	D	4618	3	18,26,27	2.75	8 (44%)	19,38,41	1.47	4 (21%)
48	PSU	w	210	48	18,21,22	1.09	1 (5%)	22,30,33	1.80	5 (22%)
48	PSU	w	866	48	18,21,22	1.05	1 (5%)	22,30,33	1.82	4 (18%)
3	A2M	D	2787	80,3	18,25,26	1.48	1 (5%)	18,36,39	1.08	1 (5%)
3	OMG	D	3899	3	18,26,27	2.71	8 (44%)	19,38,41	1.50	4 (21%)
3	PSU	D	4312	3	18,21,22	1.02	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	D	4628	3	18,21,22	1.05	1 (5%)	22,30,33	1.87	4 (18%)
3	A2M	D	1871	80,3	18,25,26	1.55	1 (5%)	18,36,39	1.15	1 (5%)
48	A2M	w	590	48	18,25,26	1.44	1 (5%)	18,36,39	1.05	1 (5%)
3	A2M	D	3830	3	18,25,26	1.48	1 (5%)	18,36,39	1.08	0
3	A2M	D	1534	80,3	18,25,26	1.42	1 (5%)	18,36,39	1.40	3 (16%)
2	1MA	B	57	2	16,25,26	0.97	1 (6%)	18,37,40	0.81	0
3	OMC	D	3841	3	19,22,23	2.81	8 (42%)	26,31,34	0.68	0
3	PSU	D	1781	3	18,21,22	1.05	1 (5%)	22,30,33	1.80	4 (18%)
3	A2M	D	2401	3	18,25,26	1.51	1 (5%)	18,36,39	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
48	PSU	w	1177	48	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
3	OMG	D	1625	80,3	18,26,27	2.78	8 (44%)	19,38,41	1.51	4 (21%)
3	OMC	D	1340	3	19,22,23	2.82	8 (42%)	26,31,34	0.69	0
3	OMC	D	2804	3	19,22,23	2.85	8 (42%)	26,31,34	0.69	0
48	OMG	w	683	48	18,26,27	2.81	8 (44%)	19,38,41	1.54	4 (21%)
3	OMC	D	3887	3	19,22,23	2.86	8 (42%)	26,31,34	0.76	0
3	5MC	D	3782	80,3	18,22,23	3.61	7 (38%)	26,32,35	1.08	2 (7%)
48	PSU	w	1238	48	18,21,22	1.05	1 (5%)	22,30,33	1.82	5 (22%)
48	A2M	w	1383	48	18,25,26	1.48	1 (5%)	18,36,39	1.21	2 (11%)
3	PSU	D	3768	3	18,21,22	1.05	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4361	3	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	D	4532	3	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
3	OMG	D	2364	3	18,26,27	2.68	8 (44%)	19,38,41	1.50	4 (21%)
3	OMG	D	2424	3	18,26,27	2.77	8 (44%)	19,38,41	1.51	4 (21%)
3	OMG	D	4623	3	18,26,27	2.72	8 (44%)	19,38,41	1.50	4 (21%)
48	PSU	w	109	48	18,21,22	1.06	1 (5%)	22,30,33	1.81	4 (18%)
48	OMG	w	509	48	18,26,27	2.88	8 (44%)	19,38,41	1.49	4 (21%)
48	OMU	w	172	48	19,22,23	2.94	8 (42%)	26,31,34	1.71	5 (19%)
3	PSU	D	3637	80,3	18,21,22	1.04	1 (5%)	22,30,33	1.90	4 (18%)
48	PSU	w	609	48	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
3	OMG	D	3627	3	18,26,27	2.73	8 (44%)	19,38,41	1.55	4 (21%)
3	A2M	D	3724	3	18,25,26	1.47	1 (5%)	18,36,39	1.02	1 (5%)
3	UR3	D	4530	3	19,22,23	2.63	7 (36%)	26,32,35	1.30	2 (7%)
48	PSU	w	1244	48	18,21,22	1.02	1 (5%)	22,30,33	1.79	4 (18%)
48	PSU	w	36	48	18,21,22	1.08	1 (5%)	22,30,33	1.86	5 (22%)
48	A2M	w	1031	48	18,25,26	1.50	1 (5%)	18,36,39	1.00	0
48	PSU	w	649	48	18,21,22	1.04	1 (5%)	22,30,33	1.85	5 (22%)
48	PSU	w	1692	48	18,21,22	1.00	1 (5%)	22,30,33	1.82	4 (18%)
48	MA6	w	1851	48	19,26,27	1.00	1 (5%)	18,38,41	1.78	3 (16%)
48	OMC	w	1391	48	19,22,23	2.93	8 (42%)	26,31,34	0.74	0
48	PSU	w	1174	48,80	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)

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
2	5MC	B	47	2	-	3/7/25/26	0/2/2/2
48	A2M	w	668	48,80	-	3/5/27/28	0/3/3/3
48	PSU	w	1625	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1677	3	-	5/7/25/26	0/2/2/2
2	5MU	B	53	2	-	2/7/25/26	0/2/2/2
3	PSU	D	3762	3	-	0/7/25/26	0/2/2/2
3	6MZ	D	4220	3	-	0/5/27/28	0/3/3/3
3	OMC	D	2351	80,3	-	1/9/27/28	0/2/2/2
48	PSU	w	119	48	-	0/7/25/26	0/2/2/2
3	UY1	D	3818	80,3	-	4/9/27/28	0/2/2/2
2	2MG	C	6	2	-	0/5/27/28	0/3/3/3
3	PSU	D	4972	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	4500	2,3	-	3/7/25/26	0/2/2/2
48	PSU	w	966	48	-	0/7/25/26	0/2/2/2
48	OMU	w	116	48	-	2/9/27/28	0/2/2/2
48	4AC	w	1842	48	-	0/11/29/30	0/2/2/2
48	A2M	w	27	48	-	1/5/27/28	0/3/3/3
48	PSU	w	1347	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4552	3	-	0/7/25/26	0/2/2/2
2	5MC	C	48	2	-	2/7/25/26	0/2/2/2
3	PSU	D	3770	3	-	1/7/25/26	0/2/2/2
3	PSU	D	4420	3	-	0/7/25/26	0/2/2/2
3	OMG	D	4228	3	-	0/5/27/28	0/3/3/3
3	PSU	D	4521	80,3	-	2/7/25/26	0/2/2/2
48	PSU	w	686	48	-	0/7/25/26	0/2/2/2
48	PSU	w	406	48	-	0/7/25/26	0/2/2/2
3	OMG	D	3944	3	-	4/5/27/28	0/3/3/3
48	B8N	w	1248	48	-	4/16/34/35	0/2/2/2
3	A2M	D	3825	3	-	0/5/27/28	0/3/3/3
3	A2M	D	1326	3	-	0/5/27/28	0/3/3/3
3	PSU	D	5001	80,3	-	0/7/25/26	0/2/2/2
3	PSU	D	1860	3	-	0/7/25/26	0/2/2/2
48	A2M	w	99	48,80	-	2/5/27/28	0/3/3/3
48	OMG	w	1490	48,80	-	3/5/27/28	0/3/3/3
3	OMU	D	2837	3	-	0/9/27/28	0/2/2/2
48	MA6	w	1850	48	-	0/7/29/30	0/3/3/3
3	OMC	D	4456	3	-	0/9/27/28	0/2/2/2
2	H2U	C	19	2	-	0/7/38/39	0/2/2/2
48	PSU	w	1045	48	-	0/7/25/26	0/2/2/2
2	1MA	C	9	2	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	w	93	48	-	0/7/25/26	0/2/2/2
3	PSU	D	3764	3	-	0/7/25/26	0/2/2/2
3	OMC	D	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3851	3	-	1/7/25/26	0/2/2/2
3	OMU	D	2415	3	-	3/9/27/28	0/2/2/2
3	PSU	D	2508	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4293	3	-	0/7/25/26	0/2/2/2
3	OMG	D	4499	2,3	-	1/5/27/28	0/3/3/3
48	PSU	w	1004	48	-	0/7/25/26	0/2/2/2
48	4AC	w	1337	48	-	0/11/29/30	0/2/2/2
3	PSU	D	3730	3	-	0/7/25/26	0/2/2/2
48	PSU	w	815	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1643	48,80	-	0/7/25/26	0/2/2/2
2	5MC	C	47	2	-	3/7/25/26	0/2/2/2
3	1MA	D	1322	3	-	0/3/25/26	0/3/3/3
3	OMG	D	4637	3	-	1/5/27/28	0/3/3/3
48	OMU	w	1326	48	-	5/9/27/28	0/2/2/2
2	H2U	B	19	2	-	0/7/38/39	0/2/2/2
3	OMU	D	1773	3	-	1/9/27/28	0/2/2/2
3	OMU	D	4498	80,3	-	0/9/27/28	0/2/2/2
2	5MU	C	53	2	-	2/7/25/26	0/2/2/2
3	OMG	D	1316	3	-	0/5/27/28	0/3/3/3
3	OMG	D	1522	3	-	0/5/27/28	0/3/3/3
3	PSU	D	3920	80,3	-	0/7/25/26	0/2/2/2
48	OMG	w	644	48	-	3/5/27/28	0/3/3/3
48	OMC	w	1703	48,80	-	2/9/27/28	0/2/2/2
3	OMU	D	3925	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4576	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1367	48	-	0/7/25/26	0/2/2/2
3	OMU	D	4227	3	-	1/9/27/28	0/2/2/2
2	5MC	B	48	2	-	2/7/25/26	0/2/2/2
2	1MA	C	57	2	-	0/3/25/26	0/3/3/3
3	A2M	D	1524	3	-	1/5/27/28	0/3/3/3
3	OMG	D	4494	3	-	1/5/27/28	0/3/3/3
48	PSU	w	822	48	-	2/7/25/26	0/2/2/2
48	PSU	w	1056	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1792	3	-	0/7/25/26	0/2/2/2
3	OMC	D	2422	80,3	-	1/9/27/28	0/2/2/2
2	2MG	B	6	2	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	w	218	48	-	0/7/25/26	0/2/2/2
48	OMG	w	436	48	-	0/5/27/28	0/3/3/3
3	PSU	D	4423	3	-	0/7/25/26	0/2/2/2
3	PSU	D	3758	3	-	0/7/25/26	0/2/2/2
2	5MC	C	38	2	-	0/7/25/26	0/2/2/2
48	PSU	w	681	48,80	-	0/7/25/26	0/2/2/2
3	A2M	D	3785	80,3	-	2/5/27/28	0/3/3/3
3	OMG	D	4370	3	-	1/5/27/28	0/3/3/3
3	A2M	D	400	3	-	0/5/27/28	0/3/3/3
3	5MC	D	4447	80,3	-	4/7/25/26	0/2/2/2
2	56B	B	34	2	-	3/6/43/44	0/4/4/4
3	OMC	D	2861	3	-	0/9/27/28	0/2/2/2
48	OMG	w	601	48	-	0/5/27/28	0/3/3/3
3	PSU	D	3715	3	-	0/7/25/26	0/2/2/2
48	PSU	w	651	48	-	0/7/25/26	0/2/2/2
3	PSU	D	3695	3	-	0/7/25/26	0/2/2/2
48	PSU	w	105	48	-	0/7/25/26	0/2/2/2
48	A2M	w	512	48	-	2/5/27/28	0/3/3/3
48	OMU	w	1288	48	-	3/9/27/28	0/2/2/2
48	OMU	w	1442	48,80	-	1/9/27/28	0/2/2/2
48	PSU	w	1445	48	-	0/7/25/26	0/2/2/2
3	PSU	D	1536	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4457	3	-	0/7/25/26	0/2/2/2
48	6MZ	w	1832	48,80	-	2/5/27/28	0/3/3/3
3	PSU	D	4471	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4431	3	-	0/7/25/26	0/2/2/2
48	PSU	w	801	48	-	0/7/25/26	0/2/2/2
3	PSU	D	4579	3	-	0/7/25/26	0/2/2/2
3	OMU	D	4620	3	-	0/9/27/28	0/2/2/2
2	5MC	B	38	2	-	0/7/25/26	0/2/2/2
3	OMC	D	3701	80,3	-	4/9/27/28	0/2/2/2
48	OMC	w	462	48	-	1/9/27/28	0/2/2/2
3	A2M	D	3760	3	-	2/5/27/28	0/3/3/3
48	PSU	w	863	48	-	0/7/25/26	0/2/2/2
48	PSU	w	572	48	-	0/7/25/26	0/2/2/2
2	PSU	C	13	2	-	0/7/25/26	0/2/2/2
48	OMG	w	1328	48	-	0/5/27/28	0/3/3/3
48	A2M	w	468	48	-	2/5/27/28	0/3/3/3
2	1MA	B	9	2	-	2/3/25/26	0/3/3/3
5	OMG	F	75	5	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	OMU	w	428	48	-	7/9/27/28	0/2/2/2
3	PSU	D	3639	3	-	0/7/25/26	0/2/2/2
48	A2M	w	484	48	-	0/5/27/28	0/3/3/3
3	PSU	D	4299	3	-	0/7/25/26	0/2/2/2
3	A2M	D	398	3	-	2/5/27/28	0/3/3/3
2	56B	C	34	2	-	3/6/43/44	0/4/4/4
48	A2M	w	1678	48	-	1/5/27/28	0/3/3/3
48	OMU	w	1804	48	-	2/9/27/28	0/2/2/2
3	OMC	D	3808	3	-	0/9/27/28	0/2/2/2
3	PSU	D	1862	3	-	0/7/25/26	0/2/2/2
48	OMU	w	121	48	-	0/9/27/28	0/2/2/2
48	A2M	w	159	48	-	2/5/27/28	0/3/3/3
2	PSU	B	13	2	-	2/7/25/26	0/2/2/2
3	PSU	D	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4353	3	-	0/7/25/26	0/2/2/2
48	OMC	w	517	48,80	-	0/9/27/28	0/2/2/2
3	PSU	D	1782	3	-	0/7/25/26	0/2/2/2
3	OMG	D	3744	3	-	0/5/27/28	0/3/3/3
3	PSU	D	1683	3	-	0/7/25/26	0/2/2/2
3	OMC	D	2365	80,3	-	0/9/27/28	0/2/2/2
48	OMU	w	627	48	-	5/9/27/28	0/2/2/2
48	A2M	w	166	48	-	2/5/27/28	0/3/3/3
48	OMU	w	799	48	-	3/9/27/28	0/2/2/2
3	OMG	D	1760	3	-	2/5/27/28	0/3/3/3
48	PSU	w	1232	48	-	0/7/25/26	0/2/2/2
3	A2M	D	2815	3	-	3/5/27/28	0/3/3/3
2	PSU	C	54	2	-	2/7/25/26	0/2/2/2
3	OMG	D	3792	3	-	0/5/27/28	0/3/3/3
48	PSU	w	1046	48	-	0/7/25/26	0/2/2/2
48	G7M	w	1639	48,2	-	2/3/25/26	0/3/3/3
3	PSU	D	4403	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	1081	48	-	0/7/25/26	0/2/2/2
3	PSU	D	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	D	2632	3	-	0/7/25/26	0/2/2/2
48	A2M	w	576	48	-	2/5/27/28	0/3/3/3
3	A2M	D	3718	3	-	0/5/27/28	0/3/3/3
48	PSU	w	34	48	-	3/7/25/26	0/2/2/2
3	PSU	D	3853	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	814	48	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	D	4523	80,3	-	0/5/27/28	0/3/3/3
3	OMC	D	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	D	4689	3	-	0/7/25/26	0/2/2/2
3	OMU	D	4306	3	-	0/9/27/28	0/2/2/2
3	OMG	D	4392	3	-	0/5/27/28	0/3/3/3
3	PSU	D	1744	80,3	-	0/7/25/26	0/2/2/2
3	OMG	D	4196	80,2,3	-	1/5/27/28	0/3/3/3
3	A2M	D	2363	80,3	-	0/5/27/28	0/3/3/3
3	PSU	D	3734	3	-	0/7/25/26	0/2/2/2
2	PSU	B	54	2	-	0/7/25/26	0/2/2/2
48	OMC	w	174	48	-	1/9/27/28	0/2/2/2
3	OMG	D	4618	3	-	0/5/27/28	0/3/3/3
48	PSU	w	210	48	-	0/7/25/26	0/2/2/2
48	PSU	w	866	48	-	0/7/25/26	0/2/2/2
3	A2M	D	2787	80,3	-	0/5/27/28	0/3/3/3
3	OMG	D	3899	3	-	0/5/27/28	0/3/3/3
3	PSU	D	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4628	3	-	0/7/25/26	0/2/2/2
3	A2M	D	1871	80,3	-	0/5/27/28	0/3/3/3
48	A2M	w	590	48	-	2/5/27/28	0/3/3/3
3	A2M	D	3830	3	-	0/5/27/28	0/3/3/3
3	A2M	D	1534	80,3	-	3/5/27/28	0/3/3/3
2	1MA	B	57	2	-	0/3/25/26	0/3/3/3
3	OMC	D	3841	3	-	0/9/27/28	0/2/2/2
3	PSU	D	1781	3	-	0/7/25/26	0/2/2/2
3	A2M	D	2401	3	-	1/5/27/28	0/3/3/3
48	PSU	w	1177	48	-	0/7/25/26	0/2/2/2
3	OMG	D	1625	80,3	-	1/5/27/28	0/3/3/3
3	OMC	D	1340	3	-	0/9/27/28	0/2/2/2
3	OMC	D	2804	3	-	0/9/27/28	0/2/2/2
48	OMG	w	683	48	-	0/5/27/28	0/3/3/3
3	OMC	D	3887	3	-	1/9/27/28	0/2/2/2
3	5MC	D	3782	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	1238	48	-	2/7/25/26	0/2/2/2
48	A2M	w	1383	48	-	0/5/27/28	0/3/3/3
3	PSU	D	3768	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4361	3	-	0/7/25/26	0/2/2/2
3	PSU	D	4532	3	-	0/7/25/26	0/2/2/2
3	OMG	D	2364	3	-	2/5/27/28	0/3/3/3
3	OMG	D	2424	3	-	2/5/27/28	0/3/3/3
3	OMG	D	4623	3	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PSU	w	109	48	-	0/7/25/26	0/2/2/2
48	OMG	w	509	48	-	1/5/27/28	0/3/3/3
48	OMU	w	172	48	-	1/9/27/28	0/2/2/2
3	PSU	D	3637	80,3	-	0/7/25/26	0/2/2/2
48	PSU	w	609	48	-	0/7/25/26	0/2/2/2
3	OMG	D	3627	3	-	0/5/27/28	0/3/3/3
3	A2M	D	3724	3	-	0/5/27/28	0/3/3/3
3	UR3	D	4530	3	-	0/7/25/26	0/2/2/2
48	PSU	w	1244	48	-	0/7/25/26	0/2/2/2
48	PSU	w	36	48	-	0/7/25/26	0/2/2/2
48	A2M	w	1031	48	-	0/5/27/28	0/3/3/3
48	PSU	w	649	48	-	0/7/25/26	0/2/2/2
48	PSU	w	1692	48	-	0/7/25/26	0/2/2/2
48	MA6	w	1851	48	-	2/7/29/30	0/3/3/3
48	OMC	w	1391	48	-	0/9/27/28	0/2/2/2
48	PSU	w	1174	48,80	-	0/7/25/26	0/2/2/2

All (760) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	53	5MU	C2-N1	10.72	1.55	1.38
2	C	53	5MU	C6-N1	10.54	1.56	1.38
2	C	53	5MU	C2-N1	10.54	1.55	1.38
2	B	53	5MU	C6-N1	10.46	1.55	1.38
2	C	48	5MC	C6-C5	9.53	1.50	1.34
2	C	47	5MC	C6-C5	9.51	1.50	1.34
2	B	48	5MC	C6-C5	9.42	1.50	1.34
2	C	38	5MC	C6-C5	9.39	1.50	1.34
2	B	47	5MC	C6-C5	9.36	1.50	1.34
2	B	38	5MC	C6-C5	9.34	1.49	1.34
3	D	4447	5MC	C6-C5	9.32	1.49	1.34
3	D	3782	5MC	C6-C5	9.17	1.49	1.34
2	C	53	5MU	C4-C5	9.15	1.60	1.44
2	B	53	5MU	C4-C5	9.13	1.59	1.44
3	D	4220	6MZ	C6-N6	7.48	1.47	1.35
2	B	48	5MC	C4-N3	7.40	1.46	1.34
2	C	53	5MU	C4-N3	-7.37	1.25	1.38
2	B	53	5MU	C4-N3	-7.36	1.25	1.38
2	C	47	5MC	C4-N3	7.30	1.46	1.34
2	B	47	5MC	C4-N3	7.30	1.46	1.34
48	w	1832	6MZ	C6-N6	7.28	1.47	1.35
2	C	38	5MC	C4-N3	7.25	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	48	5MC	C4-N3	7.24	1.46	1.34
48	w	121	OMU	C2-N1	7.16	1.49	1.38
48	w	1288	OMU	C2-N1	7.15	1.49	1.38
2	B	38	5MC	C4-N3	7.12	1.46	1.34
48	w	172	OMU	C2-N1	7.09	1.49	1.38
48	w	799	OMU	C2-N1	7.08	1.49	1.38
48	w	428	OMU	C2-N1	7.05	1.49	1.38
48	w	116	OMU	C2-N1	7.04	1.49	1.38
3	D	1773	OMU	C2-N1	7.02	1.49	1.38
2	C	34	56B	C14-C13	7.00	1.52	1.32
48	w	627	OMU	C2-N1	7.00	1.49	1.38
2	B	34	56B	C14-C13	6.98	1.52	1.32
48	w	1326	OMU	C2-N1	6.90	1.49	1.38
48	w	1804	OMU	C2-N1	6.87	1.49	1.38
3	D	3782	5MC	C4-N3	6.84	1.45	1.34
3	D	2415	OMU	C2-N1	6.84	1.49	1.38
48	w	1442	OMU	C2-N1	6.83	1.49	1.38
3	D	4227	OMU	C2-N1	6.78	1.49	1.38
48	w	1288	OMU	C2-N3	6.66	1.49	1.38
48	w	172	OMU	C2-N3	6.65	1.49	1.38
3	D	3925	OMU	C2-N1	6.64	1.49	1.38
3	D	4530	UR3	C2-N1	6.63	1.48	1.38
48	w	799	OMU	C2-N3	6.63	1.49	1.38
3	D	1773	OMU	C2-N3	6.62	1.49	1.38
48	w	121	OMU	C2-N3	6.62	1.49	1.38
48	w	428	OMU	C2-N3	6.58	1.49	1.38
48	w	116	OMU	C2-N3	6.57	1.49	1.38
3	D	4447	5MC	C4-N3	6.56	1.45	1.34
3	D	4498	OMU	C2-N1	6.55	1.49	1.38
48	w	627	OMU	C2-N3	6.54	1.49	1.38
2	C	53	5MU	C6-C5	6.51	1.45	1.34
48	w	1326	OMU	C2-N3	6.49	1.49	1.38
48	w	1442	OMU	C2-N3	6.48	1.49	1.38
2	C	47	5MC	C2-N3	6.48	1.49	1.36
2	C	48	5MC	C2-N3	6.45	1.49	1.36
2	B	48	5MC	C2-N3	6.44	1.49	1.36
2	B	47	5MC	C2-N3	6.43	1.49	1.36
2	C	38	5MC	C2-N3	6.42	1.49	1.36
48	w	1639	G7M	C2-N2	6.42	1.49	1.34
48	w	1804	OMU	C2-N3	6.42	1.49	1.38
3	D	2837	OMU	C2-N1	6.42	1.48	1.38
3	D	4306	OMU	C2-N1	6.41	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4620	OMU	C2-N1	6.41	1.48	1.38
2	B	53	5MU	C6-C5	6.38	1.45	1.34
48	w	174	OMC	C2-N3	6.32	1.49	1.36
2	B	38	5MC	C2-N3	6.32	1.49	1.36
48	w	462	OMC	C2-N3	6.29	1.49	1.36
48	w	517	OMC	C2-N3	6.24	1.49	1.36
3	D	2415	OMU	C2-N3	6.22	1.49	1.38
3	D	4227	OMU	C2-N3	6.22	1.49	1.38
3	D	3782	5MC	C2-N3	6.20	1.48	1.36
3	D	2837	OMU	C2-N3	6.17	1.49	1.38
3	D	4306	OMU	C2-N3	6.17	1.49	1.38
3	D	4620	OMU	C2-N3	6.17	1.49	1.38
3	D	4498	OMU	C2-N3	6.16	1.49	1.38
48	w	1391	OMC	C2-N3	6.13	1.48	1.36
3	D	3925	OMU	C2-N3	6.09	1.48	1.38
48	w	462	OMC	C6-C5	6.09	1.49	1.35
48	w	174	OMC	C6-C5	6.06	1.49	1.35
48	w	517	OMC	C6-C5	6.03	1.49	1.35
3	D	3887	OMC	C2-N3	6.03	1.48	1.36
2	C	34	56B	O11-C11	-6.03	1.28	1.43
3	D	2861	OMC	C2-N3	6.01	1.48	1.36
3	D	2824	OMC	C2-N3	6.00	1.48	1.36
48	w	1703	OMC	C2-N3	6.00	1.48	1.36
3	D	2422	OMC	C2-N3	5.99	1.48	1.36
2	B	34	56B	O11-C11	-5.98	1.28	1.43
48	w	509	OMG	C4-N3	5.97	1.51	1.37
3	D	4530	UR3	C6-C5	5.96	1.48	1.35
3	D	1340	OMC	C2-N3	5.95	1.48	1.36
3	D	2804	OMC	C2-N3	5.94	1.48	1.36
3	D	2351	OMC	C2-N3	5.93	1.48	1.36
3	D	3701	OMC	C2-N3	5.93	1.48	1.36
3	D	4536	OMC	C2-N3	5.92	1.48	1.36
3	D	4447	5MC	C2-N3	5.92	1.48	1.36
3	D	2365	OMC	C2-N3	5.91	1.48	1.36
48	w	428	OMU	C6-C5	5.91	1.48	1.35
48	w	1703	OMC	C6-C5	5.90	1.48	1.35
3	D	1760	OMG	C4-N3	5.90	1.51	1.37
48	w	1391	OMC	C6-C5	5.90	1.48	1.35
3	D	3808	OMC	C2-N3	5.90	1.48	1.36
3	D	3701	OMC	C6-C5	5.89	1.48	1.35
3	D	2422	OMC	C6-C5	5.86	1.48	1.35
48	w	436	OMG	C4-N3	5.86	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	1288	OMU	C6-C5	5.86	1.48	1.35
3	D	3944	OMG	C4-N3	5.85	1.51	1.37
48	w	799	OMU	C6-C5	5.85	1.48	1.35
3	D	1773	OMU	C6-C5	5.84	1.48	1.35
48	w	601	OMG	C4-N3	5.84	1.51	1.37
48	w	121	OMU	C6-C5	5.84	1.48	1.35
48	w	172	OMU	C6-C5	5.82	1.48	1.35
3	D	2861	OMC	C6-C5	5.82	1.48	1.35
48	w	627	OMU	C6-C5	5.82	1.48	1.35
48	w	644	OMG	C4-N3	5.81	1.51	1.37
3	D	4456	OMC	C2-N3	5.81	1.48	1.36
48	w	1328	OMG	C4-N3	5.80	1.51	1.37
3	D	3841	OMC	C6-C5	5.79	1.48	1.35
48	w	1490	OMG	C4-N3	5.79	1.51	1.37
3	D	3841	OMC	C2-N3	5.79	1.48	1.36
48	w	683	OMG	C4-N3	5.79	1.51	1.37
3	D	2824	OMC	C6-C5	5.78	1.48	1.35
3	D	3887	OMC	C6-C5	5.78	1.48	1.35
3	D	1625	OMG	C4-N3	5.76	1.51	1.37
48	w	116	OMU	C6-C5	5.75	1.48	1.35
5	F	75	OMG	C4-N3	5.74	1.51	1.37
3	D	2804	OMC	C6-C5	5.74	1.48	1.35
48	w	1442	OMU	C6-C5	5.74	1.48	1.35
48	w	1639	G7M	C2-N3	5.74	1.47	1.33
3	D	4456	OMC	C6-C5	5.73	1.48	1.35
3	D	3808	OMC	C6-C5	5.73	1.48	1.35
3	D	2365	OMC	C6-C5	5.72	1.48	1.35
3	D	4536	OMC	C6-C5	5.71	1.48	1.35
48	w	1326	OMU	C6-C5	5.71	1.48	1.35
3	D	4370	OMG	C4-N3	5.70	1.51	1.37
3	D	1340	OMC	C6-C5	5.69	1.48	1.35
3	D	3744	OMG	C4-N3	5.67	1.51	1.37
3	D	4637	OMG	C4-N3	5.67	1.51	1.37
3	D	4494	OMG	C4-N3	5.67	1.51	1.37
3	D	3792	OMG	C4-N3	5.67	1.51	1.37
48	w	1804	OMU	C6-C5	5.66	1.48	1.35
3	D	2415	OMU	C6-C5	5.65	1.48	1.35
3	D	2351	OMC	C6-C5	5.65	1.48	1.35
3	D	4499	OMG	C4-N3	5.65	1.51	1.37
3	D	4618	OMG	C4-N3	5.65	1.51	1.37
3	D	4228	OMG	C4-N3	5.64	1.51	1.37
3	D	4498	OMU	C6-C5	5.64	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4392	OMG	C4-N3	5.64	1.51	1.37
3	D	1316	OMG	C4-N3	5.63	1.51	1.37
3	D	3627	OMG	C4-N3	5.63	1.51	1.37
3	D	2424	OMG	C4-N3	5.63	1.51	1.37
3	D	3899	OMG	C4-N3	5.63	1.51	1.37
48	w	509	OMG	C2-N3	5.62	1.46	1.33
3	D	4196	OMG	C4-N3	5.61	1.51	1.37
3	D	4227	OMU	C6-C5	5.59	1.48	1.35
3	D	3925	OMU	C6-C5	5.58	1.48	1.35
3	D	4623	OMG	C4-N3	5.57	1.50	1.37
3	D	4620	OMU	C6-C5	5.57	1.48	1.35
3	D	4306	OMU	C6-C5	5.56	1.48	1.35
3	D	1522	OMG	C4-N3	5.54	1.50	1.37
3	D	2837	OMU	C6-C5	5.53	1.47	1.35
2	C	34	56B	C2-N3	5.53	1.46	1.33
3	D	2364	OMG	C4-N3	5.52	1.50	1.37
48	w	644	OMG	C2-N3	5.50	1.46	1.33
2	B	34	56B	C2-N3	5.49	1.46	1.33
48	w	1328	OMG	C2-N3	5.44	1.46	1.33
3	D	1760	OMG	C2-N3	5.40	1.46	1.33
48	w	601	OMG	C2-N3	5.40	1.46	1.33
3	D	1625	OMG	C2-N3	5.37	1.46	1.33
48	w	1490	OMG	C2-N3	5.34	1.46	1.33
2	B	34	56B	C11-C10	5.33	1.62	1.54
48	w	436	OMG	C2-N3	5.32	1.46	1.33
3	D	3944	OMG	C2-N3	5.32	1.46	1.33
48	w	683	OMG	C2-N3	5.32	1.46	1.33
3	D	2424	OMG	C2-N3	5.30	1.46	1.33
3	D	1524	A2M	O5'-C5'	-5.29	1.31	1.44
5	F	75	OMG	C2-N3	5.29	1.46	1.33
3	D	4494	OMG	C2-N3	5.26	1.46	1.33
48	w	509	OMG	C2-N2	5.24	1.46	1.34
2	C	34	56B	C11-C10	5.23	1.62	1.54
3	D	4370	OMG	C2-N3	5.21	1.45	1.33
3	D	3744	OMG	C2-N3	5.21	1.45	1.33
48	w	668	A2M	O5'-C5'	-5.20	1.32	1.44
3	D	4637	OMG	C2-N3	5.18	1.45	1.33
2	C	48	5MC	C6-N1	5.18	1.46	1.38
3	D	3627	OMG	C2-N3	5.18	1.45	1.33
3	D	4499	OMG	C2-N3	5.17	1.45	1.33
2	C	47	5MC	C6-N1	5.17	1.46	1.38
3	D	4618	OMG	C2-N3	5.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	48	5MC	C6-N1	5.16	1.46	1.38
3	D	1316	OMG	C2-N3	5.16	1.45	1.33
3	D	1760	OMG	C2-N2	5.16	1.46	1.34
48	w	601	OMG	C2-N2	5.16	1.46	1.34
3	D	4196	OMG	C2-N3	5.15	1.45	1.33
48	w	644	OMG	C2-N2	5.15	1.46	1.34
3	D	4228	OMG	C2-N3	5.14	1.45	1.33
3	D	3785	A2M	O5'-C5'	-5.13	1.32	1.44
3	D	3944	OMG	C2-N2	5.13	1.46	1.34
3	D	3792	OMG	C2-N3	5.12	1.45	1.33
3	D	2424	OMG	C2-N2	5.12	1.46	1.34
3	D	4392	OMG	C2-N3	5.11	1.45	1.33
48	w	174	OMC	C4-N3	5.10	1.44	1.34
3	D	2401	A2M	O5'-C5'	-5.10	1.32	1.44
48	w	1328	OMG	C2-N2	5.09	1.46	1.34
2	C	6	2MG	C4-N3	5.09	1.49	1.37
48	w	683	OMG	C2-N2	5.08	1.46	1.34
2	C	38	5MC	C6-N1	5.08	1.46	1.38
3	D	4623	OMG	C2-N3	5.08	1.45	1.33
48	w	436	OMG	C2-N2	5.08	1.46	1.34
3	D	2815	A2M	O5'-C5'	-5.07	1.32	1.44
2	B	6	2MG	C4-N3	5.07	1.49	1.37
48	w	462	OMC	C4-N3	5.07	1.44	1.34
3	D	3899	OMG	C2-N3	5.05	1.45	1.33
3	D	1522	OMG	C2-N3	5.05	1.45	1.33
2	C	6	2MG	C2-N1	5.04	1.44	1.36
5	F	75	OMG	C2-N2	5.04	1.46	1.34
3	D	400	A2M	O5'-C5'	-5.04	1.32	1.44
3	D	4618	OMG	C2-N2	5.04	1.46	1.34
2	B	47	5MC	C6-N1	5.03	1.46	1.38
48	w	484	A2M	O5'-C5'	-5.03	1.32	1.44
3	D	1625	OMG	C2-N2	5.02	1.46	1.34
48	w	517	OMC	C4-N3	5.02	1.44	1.34
48	w	1490	OMG	C2-N2	5.02	1.46	1.34
48	w	468	A2M	O5'-C5'	-5.02	1.32	1.44
3	D	4523	A2M	O5'-C5'	-5.02	1.32	1.44
3	D	1871	A2M	O5'-C5'	-5.01	1.32	1.44
3	D	3825	A2M	O5'-C5'	-5.01	1.32	1.44
3	D	2364	OMG	C2-N3	5.01	1.45	1.33
3	D	3830	A2M	O5'-C5'	-5.00	1.32	1.44
48	w	1639	G7M	C4-N3	4.99	1.49	1.37
2	B	6	2MG	C2-N1	4.99	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3744	OMG	C2-N2	4.99	1.46	1.34
2	B	38	5MC	C6-N1	4.98	1.46	1.38
3	D	4499	OMG	C2-N2	4.97	1.46	1.34
3	D	2787	A2M	O5'-C5'	-4.97	1.32	1.44
48	w	1391	OMC	C4-N3	4.96	1.44	1.34
3	D	4494	OMG	C2-N2	4.96	1.46	1.34
3	D	4623	OMG	C2-N2	4.96	1.46	1.34
48	w	1031	A2M	O5'-C5'	-4.95	1.32	1.44
3	D	3760	A2M	O5'-C5'	-4.93	1.32	1.44
48	w	174	OMC	C4-N4	4.93	1.45	1.33
3	D	3627	OMG	C2-N2	4.93	1.45	1.34
48	w	27	A2M	O5'-C5'	-4.92	1.32	1.44
48	w	1383	A2M	O5'-C5'	-4.92	1.32	1.44
3	D	1316	OMG	C2-N2	4.91	1.45	1.34
3	D	4228	OMG	C2-N2	4.90	1.45	1.34
3	D	4370	OMG	C2-N2	4.90	1.45	1.34
48	w	462	OMC	C4-N4	4.88	1.45	1.33
3	D	4637	OMG	C2-N2	4.87	1.45	1.34
48	w	159	A2M	O5'-C5'	-4.87	1.32	1.44
48	w	517	OMC	C4-N4	4.86	1.45	1.33
3	D	1326	A2M	O5'-C5'	-4.86	1.32	1.44
3	D	4196	OMG	C2-N2	4.84	1.45	1.34
3	D	3792	OMG	C2-N2	4.84	1.45	1.34
3	D	4447	5MC	C6-N1	4.84	1.46	1.38
3	D	2364	OMG	C2-N2	4.84	1.45	1.34
48	w	1703	OMC	C4-N3	4.84	1.44	1.34
3	D	4392	OMG	C2-N2	4.84	1.45	1.34
3	D	1522	OMG	C2-N2	4.83	1.45	1.34
3	D	3899	OMG	C2-N2	4.83	1.45	1.34
3	D	3782	5MC	C6-N1	4.83	1.46	1.38
48	w	166	A2M	O5'-C5'	-4.82	1.33	1.44
48	w	1391	OMC	C4-N4	4.82	1.45	1.33
2	C	34	56B	C4-N3	4.81	1.49	1.37
3	D	2804	OMC	C4-N3	4.81	1.44	1.34
3	D	3887	OMC	C4-N3	4.80	1.44	1.34
48	w	99	A2M	O5'-C5'	-4.78	1.33	1.44
3	D	3718	A2M	O5'-C5'	-4.78	1.33	1.44
48	w	512	A2M	O5'-C5'	-4.77	1.33	1.44
3	D	2824	OMC	C4-N3	4.77	1.44	1.34
2	B	34	56B	C4-N3	4.77	1.48	1.37
48	w	1703	OMC	C4-N4	4.76	1.45	1.33
3	D	398	A2M	O5'-C5'	-4.75	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2422	OMC	C4-N3	4.74	1.44	1.34
3	D	2365	OMC	C4-N3	4.72	1.44	1.34
2	C	34	56B	C2-N2	4.72	1.45	1.34
3	D	2422	OMC	C4-N4	4.71	1.45	1.33
3	D	3808	OMC	C4-N4	4.71	1.45	1.33
3	D	4456	OMC	C4-N3	4.69	1.44	1.34
3	D	4536	OMC	C4-N3	4.69	1.44	1.34
3	D	2804	OMC	C4-N4	4.69	1.45	1.33
3	D	4530	UR3	C2-N3	4.69	1.48	1.39
3	D	3724	A2M	O5'-C5'	-4.69	1.33	1.44
3	D	3701	OMC	C4-N3	4.69	1.44	1.34
3	D	3887	OMC	C4-N4	4.68	1.44	1.33
3	D	2861	OMC	C4-N4	4.68	1.44	1.33
3	D	2363	A2M	O5'-C5'	-4.68	1.33	1.44
3	D	4536	OMC	C4-N4	4.67	1.44	1.33
3	D	3701	OMC	C4-N4	4.66	1.44	1.33
3	D	2365	OMC	C4-N4	4.66	1.44	1.33
2	B	34	56B	C2-N2	4.66	1.45	1.34
3	D	1340	OMC	C4-N4	4.65	1.44	1.33
3	D	4456	OMC	C4-N4	4.65	1.44	1.33
3	D	1340	OMC	C4-N3	4.64	1.43	1.34
3	D	2861	OMC	C4-N3	4.64	1.43	1.34
48	w	1678	A2M	O5'-C5'	-4.64	1.33	1.44
3	D	3808	OMC	C4-N3	4.63	1.43	1.34
3	D	2824	OMC	C4-N4	4.63	1.44	1.33
3	D	3841	OMC	C4-N4	4.62	1.44	1.33
3	D	3841	OMC	C4-N3	4.61	1.43	1.34
3	D	2351	OMC	C4-N3	4.61	1.43	1.34
48	w	576	A2M	O5'-C5'	-4.58	1.33	1.44
48	w	590	A2M	O5'-C5'	-4.55	1.33	1.44
48	w	174	OMC	C2-N1	4.55	1.49	1.40
3	D	1534	A2M	O5'-C5'	-4.54	1.33	1.44
3	D	2351	OMC	C4-N4	4.53	1.44	1.33
48	w	517	OMC	C2-N1	4.52	1.49	1.40
48	w	462	OMC	C2-N1	4.44	1.49	1.40
2	C	48	5MC	C2-N1	4.30	1.49	1.40
48	w	1391	OMC	C2-N1	4.27	1.49	1.40
3	D	2824	OMC	C2-N1	4.21	1.49	1.40
2	B	48	5MC	C2-N1	4.21	1.49	1.40
2	C	47	5MC	C2-N1	4.20	1.49	1.40
3	D	3808	OMC	C2-N1	4.18	1.49	1.40
2	C	38	5MC	C2-N1	4.18	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2422	OMC	C2-N1	4.17	1.49	1.40
48	w	1703	OMC	C2-N1	4.16	1.49	1.40
2	B	38	5MC	C2-N1	4.15	1.49	1.40
2	B	47	5MC	C2-N1	4.14	1.49	1.40
2	C	48	5MC	C4-N4	4.14	1.44	1.34
3	D	2804	OMC	C2-N1	4.13	1.48	1.40
2	C	47	5MC	C4-N4	4.13	1.44	1.34
2	B	48	5MC	C4-N4	4.12	1.44	1.34
2	B	47	5MC	C4-N4	4.09	1.44	1.34
3	D	3701	OMC	C2-N1	4.08	1.48	1.40
3	D	2365	OMC	C2-N1	4.08	1.48	1.40
2	C	38	5MC	C4-N4	4.07	1.44	1.34
48	w	1639	G7M	C6-N1	4.07	1.43	1.37
3	D	2861	OMC	C2-N1	4.04	1.48	1.40
3	D	2351	OMC	C2-N1	4.04	1.48	1.40
48	w	509	OMG	C6-N1	4.03	1.43	1.37
3	D	4536	OMC	C2-N1	4.03	1.48	1.40
2	B	38	5MC	C4-N4	4.02	1.44	1.34
3	D	3887	OMC	C2-N1	4.02	1.48	1.40
3	D	1760	OMG	C6-N1	4.01	1.43	1.37
3	D	3841	OMC	C2-N1	3.97	1.48	1.40
3	D	1340	OMC	C2-N1	3.97	1.48	1.40
48	w	644	OMG	C6-N1	3.96	1.43	1.37
3	D	3944	OMG	C6-N1	3.94	1.43	1.37
48	w	436	OMG	C6-N1	3.94	1.43	1.37
3	D	3782	5MC	C2-N1	3.93	1.48	1.40
3	D	4456	OMC	C2-N1	3.93	1.48	1.40
3	D	4447	5MC	C2-N1	3.92	1.48	1.40
48	w	1328	OMG	C6-N1	3.92	1.43	1.37
3	D	3782	5MC	C4-N4	3.90	1.44	1.34
48	w	601	OMG	C6-N1	3.89	1.43	1.37
3	D	4447	5MC	C4-N4	3.87	1.44	1.34
48	w	683	OMG	C6-N1	3.84	1.43	1.37
48	w	644	OMG	C5-C6	3.83	1.55	1.47
3	D	1760	OMG	C5-C6	3.81	1.55	1.47
3	D	3744	OMG	C6-N1	3.78	1.43	1.37
48	w	436	OMG	C5-C6	3.76	1.55	1.47
5	F	75	OMG	C6-N1	3.75	1.43	1.37
48	w	1328	OMG	C5-C6	3.74	1.55	1.47
3	D	3944	OMG	C5-C6	3.73	1.55	1.47
3	D	2424	OMG	C6-N1	3.73	1.43	1.37
48	w	509	OMG	C5-C6	3.73	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1625	OMG	C6-N1	3.70	1.43	1.37
48	w	683	OMG	C5-C6	3.70	1.54	1.47
3	D	4499	OMG	C6-N1	3.68	1.43	1.37
3	D	4618	OMG	C6-N1	3.67	1.43	1.37
48	w	1490	OMG	C6-N1	3.65	1.43	1.37
2	C	6	2MG	C6-N1	3.64	1.43	1.37
48	w	601	OMG	C5-C6	3.64	1.54	1.47
3	D	1316	OMG	C5-C4	-3.63	1.33	1.43
3	D	4637	OMG	C6-N1	3.63	1.43	1.37
3	D	4494	OMG	C6-N1	3.61	1.43	1.37
2	B	6	2MG	C6-N1	3.60	1.43	1.37
3	D	2364	OMG	C6-N1	3.60	1.43	1.37
3	D	4618	OMG	C5-C6	3.60	1.54	1.47
3	D	4623	OMG	C6-N1	3.59	1.43	1.37
5	F	75	OMG	C5-C6	3.59	1.54	1.47
48	w	1490	OMG	C5-C6	3.58	1.54	1.47
3	D	4228	OMG	C6-N1	3.58	1.43	1.37
3	D	1522	OMG	C5-C4	-3.58	1.33	1.43
3	D	3627	OMG	C6-N1	3.57	1.43	1.37
3	D	3744	OMG	C5-C6	3.56	1.54	1.47
2	C	34	56B	C6-N1	3.55	1.43	1.37
3	D	3627	OMG	C5-C4	-3.55	1.34	1.43
3	D	4228	OMG	C5-C4	-3.55	1.34	1.43
48	w	210	PSU	C6-C5	3.54	1.39	1.35
3	D	3899	OMG	C6-N1	3.54	1.43	1.37
3	D	4370	OMG	C6-N1	3.53	1.43	1.37
3	D	2364	OMG	C5-C4	-3.53	1.34	1.43
48	w	1288	OMU	C4-N3	3.53	1.44	1.38
3	D	4637	OMG	C5-C4	-3.52	1.34	1.43
3	D	4392	OMG	C6-N1	3.52	1.43	1.37
3	D	4392	OMG	C5-C4	-3.52	1.34	1.43
48	w	172	OMU	C4-N3	3.51	1.44	1.38
3	D	3899	OMG	C5-C4	-3.51	1.34	1.43
3	D	4494	OMG	C5-C6	3.51	1.54	1.47
3	D	3792	OMG	C6-N1	3.50	1.43	1.37
3	D	3899	OMG	C5-C6	3.49	1.54	1.47
3	D	4370	OMG	C5-C4	-3.48	1.34	1.43
48	w	822	PSU	C6-C5	3.48	1.39	1.35
48	w	116	OMU	C4-N3	3.48	1.44	1.38
3	D	4499	OMG	C5-C4	-3.48	1.34	1.43
3	D	4499	OMG	C5-C6	3.47	1.54	1.47
48	w	815	PSU	C6-C5	3.47	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4196	OMG	C6-N1	3.47	1.43	1.37
3	D	2424	OMG	C5-C6	3.47	1.54	1.47
3	D	4228	OMG	C5-C6	3.46	1.54	1.47
3	D	2424	OMG	C5-C4	-3.45	1.34	1.43
3	D	4623	OMG	C5-C4	-3.45	1.34	1.43
3	D	3792	OMG	C5-C6	3.45	1.54	1.47
3	D	4196	OMG	C5-C6	3.45	1.54	1.47
2	C	54	PSU	C6-C5	3.45	1.39	1.35
3	D	1625	OMG	C5-C6	3.45	1.54	1.47
48	w	572	PSU	C6-C5	3.44	1.39	1.35
48	w	799	OMU	C4-N3	3.44	1.44	1.38
3	D	4623	OMG	C5-C6	3.43	1.54	1.47
3	D	2364	OMG	C5-C6	3.43	1.54	1.47
3	D	4196	OMG	C5-C4	-3.42	1.34	1.43
3	D	3792	OMG	C5-C4	-3.42	1.34	1.43
3	D	4637	OMG	C5-C6	3.42	1.54	1.47
3	D	4370	OMG	C5-C6	3.41	1.54	1.47
3	D	3744	OMG	C5-C4	-3.41	1.34	1.43
3	D	1773	OMU	C4-N3	3.41	1.44	1.38
3	D	3627	OMG	C5-C6	3.41	1.54	1.47
48	w	428	OMU	C4-N3	3.41	1.44	1.38
48	w	866	PSU	C6-C5	3.40	1.39	1.35
48	w	627	OMU	C4-N3	3.40	1.44	1.38
3	D	4494	OMG	C5-C4	-3.40	1.34	1.43
48	w	218	PSU	C6-C5	3.40	1.39	1.35
5	F	75	OMG	C5-C4	-3.40	1.34	1.43
3	D	1625	OMG	C5-C4	-3.39	1.34	1.43
48	w	609	PSU	C6-C5	3.39	1.39	1.35
48	w	119	PSU	C6-C5	3.38	1.39	1.35
3	D	4392	OMG	C5-C6	3.38	1.54	1.47
48	w	34	PSU	C6-C5	3.38	1.39	1.35
48	w	863	PSU	C6-C5	3.37	1.39	1.35
3	D	1522	OMG	C6-N1	3.37	1.42	1.37
3	D	1316	OMG	C6-N1	3.36	1.42	1.37
48	w	109	PSU	C6-C5	3.36	1.39	1.35
3	D	1316	OMG	C5-C6	3.35	1.54	1.47
3	D	4618	OMG	C5-C4	-3.35	1.34	1.43
48	w	121	OMU	C4-N3	3.35	1.44	1.38
2	B	34	56B	C6-N1	3.34	1.42	1.37
48	w	36	PSU	C6-C5	3.34	1.39	1.35
48	w	683	OMG	C5-C4	-3.34	1.34	1.43
3	D	1522	OMG	C5-C6	3.32	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	13	PSU	C6-C5	3.32	1.39	1.35
48	w	93	PSU	C6-C5	3.32	1.39	1.35
48	w	462	OMC	C6-N1	3.31	1.46	1.38
48	w	1442	OMU	C4-N3	3.31	1.44	1.38
48	w	1326	OMU	C4-N3	3.30	1.44	1.38
48	w	1004	PSU	C6-C5	3.30	1.39	1.35
2	C	6	2MG	C5-C6	3.30	1.54	1.47
2	B	54	PSU	C6-C5	3.29	1.39	1.35
48	w	686	PSU	C6-C5	3.28	1.39	1.35
48	w	1804	OMU	C4-N3	3.28	1.44	1.38
48	w	1639	G7M	C5-C6	3.28	1.53	1.45
48	w	801	PSU	C6-C5	3.27	1.39	1.35
3	D	3762	PSU	C6-C5	3.27	1.39	1.35
48	w	1625	PSU	C6-C5	3.27	1.39	1.35
2	B	13	PSU	C6-C5	3.27	1.39	1.35
48	w	105	PSU	C6-C5	3.26	1.39	1.35
48	w	1328	OMG	C5-C4	-3.25	1.34	1.43
48	w	601	OMG	C5-C4	-3.25	1.34	1.43
48	w	436	OMG	C5-C4	-3.25	1.34	1.43
48	w	174	OMC	C6-N1	3.25	1.45	1.38
3	D	4500	PSU	C6-C5	3.24	1.39	1.35
48	w	1232	PSU	C6-C5	3.24	1.39	1.35
2	B	6	2MG	C5-C6	3.23	1.54	1.47
48	w	649	PSU	C6-C5	3.23	1.39	1.35
48	w	814	PSU	C6-C5	3.23	1.39	1.35
48	w	1490	OMG	C5-C4	-3.23	1.34	1.43
48	w	517	OMC	C6-N1	3.21	1.45	1.38
48	w	644	OMG	C5-C4	-3.19	1.34	1.43
3	D	4532	PSU	C6-C5	3.18	1.39	1.35
3	D	3944	OMG	C5-C4	-3.17	1.35	1.43
3	D	3734	PSU	C6-C5	3.17	1.39	1.35
3	D	3768	PSU	C6-C5	3.17	1.39	1.35
3	D	3715	PSU	C6-C5	3.16	1.39	1.35
3	D	1760	OMG	C5-C4	-3.15	1.35	1.43
48	w	1244	PSU	C6-C5	3.15	1.39	1.35
3	D	4420	PSU	C6-C5	3.15	1.39	1.35
48	w	1045	PSU	C6-C5	3.14	1.39	1.35
3	D	3818	UY1	C2-N1	3.13	1.41	1.36
48	w	1445	PSU	C6-C5	3.13	1.39	1.35
3	D	4296	PSU	C6-C5	3.12	1.39	1.35
48	w	1174	PSU	C6-C5	3.12	1.39	1.35
3	D	3770	PSU	C6-C5	3.11	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	1367	PSU	C6-C5	3.11	1.38	1.35
3	D	2415	OMU	C4-N3	3.11	1.44	1.38
48	w	1238	PSU	C6-C5	3.10	1.38	1.35
3	D	4456	OMC	O2-C2	-3.10	1.18	1.23
2	C	34	56B	C5-C6	3.10	1.53	1.47
2	B	34	56B	C11-C12	3.10	1.58	1.53
48	w	1347	PSU	C6-C5	3.09	1.38	1.35
48	w	509	OMG	C5-C4	-3.08	1.35	1.43
48	w	966	PSU	C6-C5	3.08	1.38	1.35
3	D	1860	PSU	C6-C5	3.07	1.38	1.35
3	D	1781	PSU	C6-C5	3.07	1.38	1.35
48	w	1177	PSU	C6-C5	3.07	1.38	1.35
3	D	3764	PSU	C6-C5	3.06	1.38	1.35
48	w	406	PSU	C6-C5	3.05	1.38	1.35
48	w	1046	PSU	C6-C5	3.05	1.38	1.35
3	D	3841	OMC	O2-C2	-3.05	1.18	1.23
48	w	651	PSU	C6-C5	3.04	1.38	1.35
3	D	2632	PSU	C6-C5	3.04	1.38	1.35
3	D	4498	OMU	C4-N3	3.04	1.44	1.38
3	D	5010	PSU	C6-C5	3.04	1.38	1.35
3	D	2351	OMC	O2-C2	-3.04	1.18	1.23
3	D	4423	PSU	C6-C5	3.03	1.38	1.35
48	w	1391	OMC	C6-N1	3.03	1.45	1.38
3	D	3730	PSU	C6-C5	3.02	1.38	1.35
3	D	4306	OMU	O4-C4	-3.02	1.18	1.24
3	D	4536	OMC	O2-C2	-3.02	1.18	1.23
3	D	4227	OMU	C4-N3	3.02	1.44	1.38
48	w	1703	OMC	C6-N1	3.01	1.45	1.38
3	D	2861	OMC	O2-C2	-3.00	1.18	1.23
3	D	2861	OMC	C6-N1	3.00	1.45	1.38
3	D	2365	OMC	O2-C2	-2.99	1.18	1.23
3	D	3925	OMU	O4-C4	-2.99	1.18	1.24
3	D	2837	OMU	O4-C4	-2.99	1.18	1.24
3	D	3701	OMC	C6-N1	2.98	1.45	1.38
3	D	4552	PSU	C6-C5	2.98	1.38	1.35
3	D	3925	OMU	O2-C2	-2.98	1.17	1.23
3	D	1744	PSU	C6-C5	2.98	1.38	1.35
2	C	34	56B	C11-C12	2.97	1.58	1.53
3	D	3887	OMC	C6-N1	2.97	1.45	1.38
3	D	1340	OMC	O2-C2	-2.97	1.18	1.23
3	D	2422	OMC	C6-N1	2.97	1.45	1.38
3	D	4306	OMU	O2-C2	-2.97	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2824	OMC	C6-N1	2.97	1.45	1.38
3	D	2824	OMC	O2-C2	-2.97	1.18	1.23
3	D	3887	OMC	O2-C2	-2.97	1.18	1.23
48	w	681	PSU	C6-C5	2.96	1.38	1.35
3	D	4689	PSU	C6-C5	2.96	1.38	1.35
3	D	4972	PSU	C6-C5	2.96	1.38	1.35
3	D	4456	OMC	C6-N1	2.96	1.45	1.38
3	D	2804	OMC	C6-N1	2.95	1.45	1.38
48	w	1703	OMC	O2-C2	-2.95	1.18	1.23
3	D	5001	PSU	C6-C5	2.95	1.38	1.35
3	D	3853	PSU	C6-C5	2.95	1.38	1.35
3	D	4293	PSU	C6-C5	2.95	1.38	1.35
3	D	3808	OMC	O2-C2	-2.95	1.18	1.23
3	D	1340	OMC	C6-N1	2.95	1.45	1.38
48	w	1643	PSU	C6-C5	2.95	1.38	1.35
3	D	4628	PSU	C6-C5	2.95	1.38	1.35
48	w	1056	PSU	C6-C5	2.95	1.38	1.35
3	D	4620	OMU	C4-N3	2.94	1.43	1.38
3	D	4620	OMU	O2-C2	-2.94	1.17	1.23
3	D	4471	PSU	C6-C5	2.94	1.38	1.35
3	D	4620	OMU	O4-C4	-2.94	1.18	1.24
3	D	3695	PSU	C6-C5	2.94	1.38	1.35
3	D	2422	OMC	O2-C2	-2.94	1.18	1.23
3	D	4306	OMU	C4-N3	2.93	1.43	1.38
3	D	4312	PSU	C6-C5	2.93	1.38	1.35
3	D	2365	OMC	C6-N1	2.93	1.45	1.38
3	D	4498	OMU	O4-C4	-2.93	1.18	1.24
3	D	2508	PSU	C6-C5	2.93	1.38	1.35
3	D	1792	PSU	C6-C5	2.93	1.38	1.35
3	D	4227	OMU	O4-C4	-2.92	1.18	1.24
3	D	1862	PSU	C6-C5	2.91	1.38	1.35
3	D	4403	PSU	C6-C5	2.91	1.38	1.35
48	w	1851	MA6	C5-C4	-2.91	1.33	1.40
3	D	4431	PSU	C6-C5	2.91	1.38	1.35
3	D	4576	PSU	C6-C5	2.91	1.38	1.35
3	D	2837	OMU	C4-N3	2.91	1.43	1.38
3	D	3841	OMC	C6-N1	2.90	1.45	1.38
3	D	4536	OMC	C6-N1	2.90	1.45	1.38
3	D	4442	PSU	C6-C5	2.90	1.38	1.35
3	D	4353	PSU	C6-C5	2.90	1.38	1.35
3	D	2804	OMC	O2-C2	-2.90	1.18	1.23
3	D	4498	OMU	O2-C2	-2.90	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4361	PSU	C6-C5	2.88	1.38	1.35
3	D	3925	OMU	C4-N3	2.88	1.43	1.38
3	D	4227	OMU	O2-C2	-2.88	1.17	1.23
3	D	2351	OMC	C6-N1	2.88	1.44	1.38
3	D	2415	OMU	O4-C4	-2.87	1.18	1.24
3	D	4579	PSU	C6-C5	2.87	1.38	1.35
3	D	4457	PSU	C6-C5	2.87	1.38	1.35
3	D	4521	PSU	C6-C5	2.87	1.38	1.35
3	D	2837	OMU	O2-C2	-2.87	1.17	1.23
3	D	1782	PSU	C6-C5	2.86	1.38	1.35
2	B	34	56B	C5-C6	2.86	1.53	1.47
3	D	3808	OMC	C6-N1	2.84	1.44	1.38
3	D	4299	PSU	C6-C5	2.82	1.38	1.35
48	w	1692	PSU	C6-C5	2.82	1.38	1.35
3	D	3637	PSU	C6-C5	2.82	1.38	1.35
48	w	1639	G7M	C2-N1	2.82	1.44	1.37
48	w	1081	PSU	C6-C5	2.82	1.38	1.35
3	D	3639	PSU	C6-C5	2.81	1.38	1.35
3	D	1683	PSU	C6-C5	2.81	1.38	1.35
3	D	3701	OMC	O2-C2	-2.80	1.18	1.23
3	D	2415	OMU	O2-C2	-2.79	1.17	1.23
48	w	1326	OMU	O2-C2	-2.79	1.17	1.23
3	D	3920	PSU	C6-C5	2.79	1.38	1.35
3	D	4530	UR3	C6-N1	2.79	1.44	1.38
3	D	4392	OMG	O6-C6	-2.79	1.17	1.23
2	C	57	1MA	C2-N1	2.79	1.41	1.35
2	B	57	1MA	C2-N1	2.79	1.41	1.35
2	C	9	1MA	C2-N1	2.78	1.41	1.35
48	w	1850	MA6	C5-C4	-2.78	1.33	1.40
48	w	1391	OMC	O2-C2	-2.77	1.18	1.23
48	w	1326	OMU	O4-C4	-2.76	1.19	1.24
3	D	3758	PSU	C6-C5	2.75	1.38	1.35
3	D	4447	5MC	O2-C2	-2.75	1.18	1.23
3	D	3851	PSU	C6-C5	2.74	1.38	1.35
48	w	1804	OMU	O4-C4	-2.74	1.19	1.24
3	D	1522	OMG	O6-C6	-2.74	1.17	1.23
48	w	1442	OMU	O4-C4	-2.74	1.19	1.24
48	w	116	OMU	O4-C4	-2.73	1.19	1.24
3	D	1536	PSU	C6-C5	2.73	1.38	1.35
48	w	517	OMC	O2-C2	-2.71	1.18	1.23
2	C	34	56B	C2-N1	2.71	1.44	1.37
2	B	19	H2U	C2-N3	-2.71	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3899	OMG	O6-C6	-2.70	1.17	1.23
3	D	1316	OMG	O6-C6	-2.70	1.17	1.23
48	w	121	OMU	O4-C4	-2.70	1.19	1.24
48	w	462	OMC	O2-C2	-2.69	1.18	1.23
48	w	1442	OMU	O2-C2	-2.69	1.18	1.23
3	D	4228	OMG	O6-C6	-2.69	1.17	1.23
3	D	4370	OMG	O6-C6	-2.69	1.17	1.23
2	C	19	H2U	C2-N3	-2.68	1.33	1.38
3	D	4494	OMG	O6-C6	-2.68	1.17	1.23
48	w	509	OMG	C2-N1	2.68	1.44	1.37
48	w	799	OMU	O4-C4	-2.66	1.19	1.24
48	w	428	OMU	O4-C4	-2.66	1.19	1.24
48	w	627	OMU	O4-C4	-2.65	1.19	1.24
3	D	3627	OMG	O6-C6	-2.65	1.17	1.23
48	w	172	OMU	O4-C4	-2.65	1.19	1.24
2	B	34	56B	C5-C4	-2.65	1.37	1.40
48	w	1804	OMU	O2-C2	-2.65	1.18	1.23
48	w	428	OMU	O2-C2	-2.64	1.18	1.23
48	w	1832	6MZ	C5-C4	-2.63	1.34	1.40
3	D	1773	OMU	O2-C2	-2.63	1.18	1.23
2	B	9	1MA	C2-N1	2.63	1.40	1.35
3	D	3744	OMG	O6-C6	-2.62	1.18	1.23
3	D	4623	OMG	O6-C6	-2.62	1.18	1.23
3	D	4499	OMG	O6-C6	-2.61	1.18	1.23
3	D	1773	OMU	O4-C4	-2.61	1.19	1.24
48	w	121	OMU	O2-C2	-2.61	1.18	1.23
3	D	4220	6MZ	C5-C4	-2.60	1.34	1.40
3	D	1677	PSU	C6-C5	2.60	1.38	1.35
48	w	1288	OMU	O4-C4	-2.60	1.19	1.24
48	w	116	OMU	O2-C2	-2.60	1.18	1.23
3	D	4196	OMG	O6-C6	-2.60	1.18	1.23
2	B	34	56B	C2-N1	2.59	1.44	1.37
48	w	1288	OMU	O2-C2	-2.59	1.18	1.23
3	D	4618	OMG	O6-C6	-2.59	1.18	1.23
3	D	3792	OMG	O6-C6	-2.58	1.18	1.23
48	w	174	OMC	O2-C2	-2.58	1.18	1.23
3	D	4637	OMG	O6-C6	-2.57	1.18	1.23
3	D	2364	OMG	O6-C6	-2.57	1.18	1.23
2	B	19	H2U	C4-N3	-2.57	1.33	1.37
48	w	627	OMU	O2-C2	-2.55	1.18	1.23
48	w	799	OMU	O2-C2	-2.55	1.18	1.23
3	D	1760	OMG	C2-N1	2.54	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	668	A2M	O4'-C4'	-2.54	1.39	1.45
48	w	644	OMG	C2-N1	2.53	1.43	1.37
3	D	1625	OMG	O6-C6	-2.53	1.18	1.23
2	B	6	2MG	C5-C4	-2.52	1.36	1.43
48	w	1490	OMG	O6-C6	-2.52	1.18	1.23
48	w	172	OMU	O2-C2	-2.52	1.18	1.23
3	D	2424	OMG	O6-C6	-2.51	1.18	1.23
2	C	19	H2U	C4-N3	-2.51	1.33	1.37
48	w	462	OMC	C5-C4	2.51	1.48	1.42
48	w	517	OMC	C5-C4	2.51	1.48	1.42
48	w	174	OMC	C5-C4	2.50	1.48	1.42
48	w	683	OMG	O6-C6	-2.50	1.18	1.23
48	w	1328	OMG	C2-N1	2.49	1.43	1.37
3	D	3944	OMG	C2-N1	2.49	1.43	1.37
48	w	601	OMG	C2-N1	2.49	1.43	1.37
48	w	601	OMG	O6-C6	-2.48	1.18	1.23
2	C	6	2MG	C5-C4	-2.47	1.36	1.43
48	w	436	OMG	C2-N1	2.47	1.43	1.37
5	F	75	OMG	O6-C6	-2.46	1.18	1.23
3	D	4530	UR3	O4-C4	-2.45	1.18	1.23
48	w	683	OMG	C2-N1	2.44	1.43	1.37
48	w	436	OMG	O6-C6	-2.43	1.18	1.23
2	C	34	56B	C5-C4	-2.42	1.37	1.40
3	D	1524	A2M	O4'-C4'	-2.41	1.39	1.45
3	D	4530	UR3	O2-C2	-2.40	1.18	1.22
2	B	34	56B	O6-C6	-2.39	1.18	1.23
3	D	3782	5MC	O2-C2	-2.39	1.19	1.23
48	w	1328	OMG	O6-C6	-2.39	1.18	1.23
3	D	3944	OMG	O6-C6	-2.38	1.18	1.23
2	B	38	5MC	O2-C2	-2.38	1.19	1.23
3	D	2424	OMG	C2-N1	2.38	1.43	1.37
3	D	3744	OMG	C2-N1	2.37	1.43	1.37
3	D	4618	OMG	C2-N1	2.37	1.43	1.37
48	w	644	OMG	O6-C6	-2.36	1.18	1.23
3	D	4499	OMG	C2-N1	2.36	1.43	1.37
5	F	75	OMG	C2-N1	2.35	1.43	1.37
2	B	48	5MC	O2-C2	-2.34	1.19	1.23
3	D	3701	OMC	C5-C4	2.33	1.48	1.42
48	w	509	OMG	O6-C6	-2.33	1.18	1.23
48	w	1391	OMC	C5-C4	2.33	1.48	1.42
3	D	1760	OMG	O6-C6	-2.32	1.18	1.23
3	D	4623	OMG	C2-N1	2.32	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	38	5MC	O2-C2	-2.32	1.19	1.23
3	D	1625	OMG	C2-N1	2.30	1.43	1.37
2	B	47	5MC	O2-C2	-2.28	1.19	1.23
3	D	4494	OMG	C2-N1	2.28	1.43	1.37
2	C	34	56B	O6-C6	-2.28	1.18	1.23
48	w	1490	OMG	C2-N1	2.27	1.43	1.37
2	C	47	5MC	O2-C2	-2.26	1.19	1.23
3	D	3899	OMG	C2-N1	2.26	1.43	1.37
48	w	1639	G7M	O6-C6	-2.26	1.18	1.23
48	w	1703	OMC	C5-C4	2.25	1.48	1.42
3	D	3792	OMG	C2-N1	2.24	1.43	1.37
3	D	2364	OMG	C2-N1	2.24	1.43	1.37
3	D	3627	OMG	C2-N1	2.24	1.43	1.37
3	D	3808	OMC	C5-C4	2.23	1.48	1.42
3	D	2422	OMC	C5-C4	2.23	1.48	1.42
2	C	48	5MC	O2-C2	-2.23	1.19	1.23
3	D	3887	OMC	C5-C4	2.22	1.48	1.42
3	D	4228	OMG	C2-N1	2.22	1.43	1.37
2	C	48	5MC	CM5-C5	2.22	1.56	1.50
3	D	3785	A2M	O4'-C1'	-2.22	1.38	1.41
2	B	48	5MC	CM5-C5	2.21	1.56	1.50
2	B	47	5MC	CM5-C5	2.21	1.56	1.50
2	C	38	5MC	CM5-C5	2.20	1.56	1.50
3	D	4637	OMG	C2-N1	2.20	1.43	1.37
3	D	2824	OMC	C5-C4	2.20	1.48	1.42
3	D	4196	OMG	C2-N1	2.19	1.43	1.37
2	C	47	5MC	CM5-C5	2.19	1.56	1.50
3	D	4370	OMG	C2-N1	2.19	1.43	1.37
2	B	38	5MC	CM5-C5	2.19	1.56	1.50
3	D	1522	OMG	C2-N1	2.18	1.43	1.37
3	D	4456	OMC	C5-C4	2.18	1.47	1.42
3	D	2365	OMC	C5-C4	2.17	1.47	1.42
3	D	2861	OMC	C5-C4	2.17	1.47	1.42
3	D	2804	OMC	C5-C4	2.16	1.47	1.42
48	w	1288	OMU	C5-C4	2.15	1.48	1.43
3	D	3818	UY1	O4'-C1'	-2.15	1.40	1.43
3	D	3841	OMC	C5-C4	2.15	1.47	1.42
48	w	428	OMU	C5-C4	2.15	1.48	1.43
3	D	4536	OMC	C5-C4	2.15	1.47	1.42
3	D	4392	OMG	C2-N1	2.15	1.43	1.37
48	w	1832	6MZ	C2-N3	2.14	1.35	1.32
3	D	1316	OMG	C2-N1	2.14	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	w	1288	OMU	C6-N1	2.12	1.43	1.38
48	w	121	OMU	C6-N1	2.11	1.43	1.38
3	D	4523	A2M	O4'-C4'	-2.11	1.40	1.45
48	w	1326	OMU	C6-N1	2.10	1.43	1.38
3	D	2363	A2M	O4'-C4'	-2.10	1.40	1.45
2	C	53	5MU	O2-C2	-2.10	1.19	1.23
3	D	1773	OMU	C5-C4	2.09	1.48	1.43
48	w	799	OMU	C5-C4	2.08	1.48	1.43
48	w	627	OMU	C5-C4	2.08	1.48	1.43
3	D	1683	PSU	C4-C5	-2.08	1.38	1.44
48	w	172	OMU	C6-N1	2.08	1.43	1.38
3	D	1340	OMC	C5-C4	2.07	1.47	1.42
48	w	172	OMU	C5-C4	2.07	1.48	1.43
48	w	799	OMU	C6-N1	2.07	1.43	1.38
48	w	428	OMU	C6-N1	2.06	1.43	1.38
3	D	1677	PSU	O4'-C1'	-2.06	1.41	1.43
3	D	1773	OMU	C6-N1	2.06	1.43	1.38
2	B	34	56B	C5-C7	-2.04	1.36	1.39
3	D	4293	PSU	C4-C5	-2.03	1.38	1.44
3	D	1536	PSU	C4-C5	-2.03	1.38	1.44
48	w	116	OMU	C5-C4	2.02	1.48	1.43
48	w	121	OMU	C5-C4	2.01	1.48	1.43
3	D	4530	UR3	C5-C4	2.01	1.49	1.43
48	w	116	OMU	C6-N1	2.01	1.42	1.38

All (691) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	34	56B	C8-N9-C1'	23.29	146.11	125.48
2	B	34	56B	C8-N9-C1'	22.82	145.70	125.48
2	B	53	5MU	C5-C4-N3	12.26	125.77	115.31
2	C	53	5MU	C5-C4-N3	12.00	125.55	115.31
2	C	53	5MU	C5-C6-N1	-9.91	113.14	123.34
2	B	53	5MU	C5-C6-N1	-9.76	113.29	123.34
2	B	34	56B	C5-C6-N1	5.95	120.39	115.36
48	w	1851	MA6	N3-C2-N1	-5.90	119.46	128.68
3	D	2415	OMU	C4-N3-C2	-5.82	118.91	126.58
2	C	34	56B	C5-C6-N1	5.80	120.27	115.36
3	D	4220	6MZ	N3-C2-N1	-5.77	119.66	128.68
3	D	3925	OMU	C4-N3-C2	-5.66	119.12	126.58
3	D	2837	OMU	C4-N3-C2	-5.63	119.15	126.58
48	w	1832	6MZ	N3-C2-N1	-5.57	119.97	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1850	MA6	N3-C2-N1	-5.56	119.98	128.68
3	D	4498	OMU	C4-N3-C2	-5.50	119.32	126.58
3	D	4306	OMU	C4-N3-C2	-5.47	119.36	126.58
3	D	4227	OMU	C4-N3-C2	-5.43	119.42	126.58
48	w	1804	OMU	C4-N3-C2	-5.38	119.49	126.58
3	D	4620	OMU	C4-N3-C2	-5.34	119.54	126.58
48	w	627	OMU	C4-N3-C2	-5.32	119.56	126.58
48	w	428	OMU	C4-N3-C2	-5.28	119.61	126.58
48	w	172	OMU	C4-N3-C2	-5.26	119.64	126.58
48	w	1442	OMU	C4-N3-C2	-5.25	119.65	126.58
48	w	799	OMU	C4-N3-C2	-5.23	119.69	126.58
48	w	116	OMU	C4-N3-C2	-5.17	119.76	126.58
3	D	1773	OMU	C4-N3-C2	-5.15	119.79	126.58
48	w	1288	OMU	C4-N3-C2	-5.14	119.80	126.58
3	D	1683	PSU	N1-C2-N3	5.12	120.93	115.13
3	D	4220	6MZ	C2-N1-C6	5.08	120.95	116.59
2	B	53	5MU	O4-C4-C5	-5.08	119.02	124.90
3	D	3637	PSU	N1-C2-N3	5.00	120.80	115.13
48	w	1326	OMU	C4-N3-C2	-4.99	120.00	126.58
2	C	53	5MU	O4-C4-C5	-4.97	119.14	124.90
48	w	121	OMU	C4-N3-C2	-4.96	120.04	126.58
3	D	3637	PSU	C4-N3-C2	-4.91	119.26	126.34
3	D	4521	PSU	C4-N3-C2	-4.91	119.27	126.34
3	D	1536	PSU	C4-N3-C2	-4.90	119.28	126.34
2	B	13	PSU	N1-C2-N3	4.89	120.67	115.13
48	w	681	PSU	C4-N3-C2	-4.89	119.30	126.34
3	D	4628	PSU	N1-C2-N3	4.87	120.65	115.13
3	D	1862	PSU	N1-C2-N3	4.87	120.65	115.13
3	D	4403	PSU	N1-C2-N3	4.86	120.64	115.13
48	w	681	PSU	N1-C2-N3	4.85	120.62	115.13
48	w	651	PSU	C4-N3-C2	-4.84	119.36	126.34
3	D	1683	PSU	C4-N3-C2	-4.83	119.38	126.34
3	D	3851	PSU	N1-C2-N3	4.83	120.60	115.13
3	D	1782	PSU	C4-N3-C2	-4.83	119.38	126.34
3	D	4530	UR3	C4-N3-C2	-4.83	120.02	124.56
48	w	815	PSU	C4-N3-C2	-4.82	119.39	126.34
3	D	4431	PSU	N1-C2-N3	4.81	120.58	115.13
3	D	3851	PSU	C4-N3-C2	-4.81	119.41	126.34
3	D	1860	PSU	N1-C2-N3	4.81	120.58	115.13
3	D	3695	PSU	C4-N3-C2	-4.80	119.42	126.34
3	D	5010	PSU	C4-N3-C2	-4.80	119.42	126.34
3	D	1862	PSU	C4-N3-C2	-4.80	119.42	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1367	PSU	C4-N3-C2	-4.80	119.42	126.34
3	D	4521	PSU	N1-C2-N3	4.80	120.57	115.13
3	D	1536	PSU	N1-C2-N3	4.79	120.56	115.13
3	D	3920	PSU	C4-N3-C2	-4.79	119.44	126.34
3	D	5010	PSU	N1-C2-N3	4.78	120.55	115.13
48	w	1045	PSU	C4-N3-C2	-4.78	119.45	126.34
3	D	4431	PSU	C4-N3-C2	-4.78	119.45	126.34
3	D	1677	PSU	C4-N3-C2	-4.78	119.45	126.34
3	D	3695	PSU	N1-C2-N3	4.78	120.54	115.13
3	D	4353	PSU	C4-N3-C2	-4.77	119.47	126.34
3	D	4299	PSU	N1-C2-N3	4.77	120.53	115.13
48	w	406	PSU	C4-N3-C2	-4.77	119.47	126.34
3	D	3770	PSU	N1-C2-N3	4.77	120.53	115.13
48	w	1692	PSU	C4-N3-C2	-4.76	119.47	126.34
3	D	3920	PSU	N1-C2-N3	4.76	120.53	115.13
3	D	2508	PSU	C4-N3-C2	-4.76	119.48	126.34
3	D	4628	PSU	C4-N3-C2	-4.76	119.48	126.34
3	D	4403	PSU	C4-N3-C2	-4.76	119.48	126.34
3	D	4457	PSU	C4-N3-C2	-4.76	119.48	126.34
3	D	4576	PSU	C4-N3-C2	-4.76	119.48	126.34
48	w	814	PSU	C4-N3-C2	-4.74	119.50	126.34
2	C	53	5MU	C4-N3-C2	-4.74	121.21	127.35
3	D	4442	PSU	N1-C2-N3	4.74	120.50	115.13
3	D	4353	PSU	N1-C2-N3	4.74	120.50	115.13
3	D	4972	PSU	N1-C2-N3	4.74	120.50	115.13
48	w	1367	PSU	N1-C2-N3	4.74	120.50	115.13
3	D	3715	PSU	C4-N3-C2	-4.74	119.52	126.34
48	w	1347	PSU	C4-N3-C2	-4.73	119.52	126.34
3	D	4552	PSU	N1-C2-N3	4.73	120.49	115.13
48	w	572	PSU	C4-N3-C2	-4.73	119.52	126.34
3	D	1744	PSU	C4-N3-C2	-4.73	119.53	126.34
3	D	3758	PSU	C4-N3-C2	-4.73	119.53	126.34
48	w	1081	PSU	C4-N3-C2	-4.73	119.53	126.34
3	D	4689	PSU	N1-C2-N3	4.73	120.48	115.13
3	D	1792	PSU	C4-N3-C2	-4.72	119.53	126.34
48	w	93	PSU	C4-N3-C2	-4.72	119.53	126.34
3	D	1782	PSU	N1-C2-N3	4.72	120.48	115.13
3	D	4442	PSU	C4-N3-C2	-4.72	119.54	126.34
48	w	1056	PSU	C4-N3-C2	-4.72	119.54	126.34
3	D	4972	PSU	C4-N3-C2	-4.72	119.54	126.34
48	w	649	PSU	N1-C2-N3	4.71	120.47	115.13
48	w	1177	PSU	C4-N3-C2	-4.71	119.55	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3730	PSU	C4-N3-C2	-4.70	119.56	126.34
48	w	651	PSU	N1-C2-N3	4.70	120.46	115.13
48	w	1004	PSU	N1-C2-N3	4.70	120.46	115.13
3	D	4312	PSU	C4-N3-C2	-4.70	119.57	126.34
48	w	686	PSU	N1-C2-N3	4.70	120.45	115.13
3	D	1860	PSU	C4-N3-C2	-4.70	119.57	126.34
3	D	4293	PSU	C4-N3-C2	-4.70	119.57	126.34
48	w	649	PSU	C4-N3-C2	-4.70	119.57	126.34
3	D	4312	PSU	N1-C2-N3	4.69	120.45	115.13
3	D	3715	PSU	N1-C2-N3	4.69	120.45	115.13
3	D	4579	PSU	N1-C2-N3	4.69	120.45	115.13
48	w	1046	PSU	N1-C2-N3	4.69	120.45	115.13
3	D	4293	PSU	N1-C2-N3	4.69	120.44	115.13
3	D	1781	PSU	C4-N3-C2	-4.69	119.58	126.34
3	D	5001	PSU	C4-N3-C2	-4.69	119.59	126.34
3	D	4361	PSU	C4-N3-C2	-4.68	119.59	126.34
2	C	54	PSU	C4-N3-C2	-4.68	119.59	126.34
2	B	53	5MU	C4-N3-C2	-4.68	121.29	127.35
48	w	863	PSU	N1-C2-N3	4.68	120.43	115.13
3	D	3734	PSU	N1-C2-N3	4.68	120.43	115.13
3	D	4500	PSU	N1-C2-N3	4.68	120.43	115.13
3	D	4576	PSU	N1-C2-N3	4.68	120.43	115.13
48	w	1692	PSU	N1-C2-N3	4.68	120.43	115.13
48	w	866	PSU	C4-N3-C2	-4.68	119.60	126.34
48	w	1045	PSU	N1-C2-N3	4.68	120.43	115.13
48	w	36	PSU	N1-C2-N3	4.68	120.43	115.13
3	D	4532	PSU	N1-C2-N3	4.67	120.42	115.13
48	w	815	PSU	N1-C2-N3	4.67	120.42	115.13
3	D	3764	PSU	N1-C2-N3	4.67	120.42	115.13
48	w	1174	PSU	C4-N3-C2	-4.67	119.61	126.34
3	D	1744	PSU	N1-C2-N3	4.67	120.42	115.13
3	D	4299	PSU	C4-N3-C2	-4.67	119.61	126.34
48	w	1244	PSU	C4-N3-C2	-4.67	119.61	126.34
48	w	1046	PSU	C4-N3-C2	-4.67	119.61	126.34
3	D	4361	PSU	N1-C2-N3	4.67	120.42	115.13
3	D	3734	PSU	C4-N3-C2	-4.66	119.62	126.34
48	w	406	PSU	N1-C2-N3	4.66	120.41	115.13
3	D	4296	PSU	N1-C2-N3	4.65	120.40	115.13
3	D	4423	PSU	N1-C2-N3	4.65	120.40	115.13
3	D	2508	PSU	N1-C2-N3	4.65	120.40	115.13
3	D	4423	PSU	C4-N3-C2	-4.65	119.64	126.34
48	w	1445	PSU	C4-N3-C2	-4.65	119.64	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1238	PSU	C4-N3-C2	-4.65	119.65	126.34
3	D	4457	PSU	N1-C2-N3	4.64	120.38	115.13
3	D	3764	PSU	C4-N3-C2	-4.64	119.66	126.34
3	D	3762	PSU	N1-C2-N3	4.64	120.38	115.13
3	D	4579	PSU	C4-N3-C2	-4.64	119.66	126.34
48	w	863	PSU	C4-N3-C2	-4.64	119.66	126.34
2	B	13	PSU	C4-N3-C2	-4.64	119.66	126.34
48	w	105	PSU	N1-C2-N3	4.63	120.38	115.13
48	w	1238	PSU	N1-C2-N3	4.63	120.38	115.13
3	D	2632	PSU	C4-N3-C2	-4.63	119.67	126.34
48	w	1232	PSU	N1-C2-N3	4.63	120.38	115.13
48	w	686	PSU	C4-N3-C2	-4.63	119.67	126.34
48	w	1056	PSU	N1-C2-N3	4.63	120.38	115.13
48	w	966	PSU	N1-C2-N3	4.63	120.37	115.13
3	D	4471	PSU	N1-C2-N3	4.63	120.37	115.13
3	D	4420	PSU	C4-N3-C2	-4.63	119.67	126.34
48	w	210	PSU	C4-N3-C2	-4.63	119.67	126.34
3	D	4471	PSU	C4-N3-C2	-4.62	119.68	126.34
3	D	4689	PSU	C4-N3-C2	-4.62	119.68	126.34
3	D	4500	PSU	C4-N3-C2	-4.62	119.68	126.34
48	w	109	PSU	N1-C2-N3	4.62	120.37	115.13
48	w	1625	PSU	C4-N3-C2	-4.62	119.68	126.34
48	w	1177	PSU	N1-C2-N3	4.62	120.36	115.13
3	D	2632	PSU	N1-C2-N3	4.61	120.36	115.13
48	w	1643	PSU	N1-C2-N3	4.61	120.36	115.13
48	w	966	PSU	C4-N3-C2	-4.61	119.69	126.34
48	w	1232	PSU	C4-N3-C2	-4.61	119.70	126.34
3	D	1781	PSU	N1-C2-N3	4.61	120.35	115.13
3	D	4552	PSU	C4-N3-C2	-4.60	119.70	126.34
3	D	3768	PSU	C4-N3-C2	-4.60	119.71	126.34
48	w	1004	PSU	C4-N3-C2	-4.60	119.71	126.34
3	D	3768	PSU	N1-C2-N3	4.60	120.34	115.13
3	D	4532	PSU	C4-N3-C2	-4.60	119.72	126.34
2	C	54	PSU	N1-C2-N3	4.59	120.33	115.13
3	D	3770	PSU	C4-N3-C2	-4.59	119.73	126.34
48	w	1347	PSU	N1-C2-N3	4.59	120.33	115.13
48	w	105	PSU	C4-N3-C2	-4.58	119.74	126.34
48	w	1625	PSU	N1-C2-N3	4.58	120.32	115.13
3	D	5001	PSU	N1-C2-N3	4.58	120.32	115.13
48	w	609	PSU	N1-C2-N3	4.58	120.32	115.13
2	C	13	PSU	C4-N3-C2	-4.58	119.74	126.34
2	B	54	PSU	C4-N3-C2	-4.58	119.75	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	801	PSU	N1-C2-N3	4.57	120.31	115.13
3	D	3639	PSU	C4-N3-C2	-4.57	119.75	126.34
3	D	3730	PSU	N1-C2-N3	4.57	120.30	115.13
3	D	1677	PSU	N1-C2-N3	4.56	120.30	115.13
3	D	3762	PSU	C4-N3-C2	-4.56	119.77	126.34
48	w	866	PSU	N1-C2-N3	4.56	120.30	115.13
48	w	1643	PSU	C4-N3-C2	-4.56	119.77	126.34
48	w	801	PSU	C4-N3-C2	-4.56	119.77	126.34
48	w	1081	PSU	N1-C2-N3	4.55	120.28	115.13
3	D	3853	PSU	N1-C2-N3	4.55	120.28	115.13
3	D	3639	PSU	N1-C2-N3	4.55	120.28	115.13
48	w	1445	PSU	N1-C2-N3	4.55	120.28	115.13
3	D	4296	PSU	C4-N3-C2	-4.54	119.80	126.34
3	D	3853	PSU	C4-N3-C2	-4.54	119.80	126.34
48	w	109	PSU	C4-N3-C2	-4.53	119.81	126.34
48	w	218	PSU	C4-N3-C2	-4.53	119.82	126.34
48	w	1244	PSU	N1-C2-N3	4.52	120.26	115.13
3	D	3758	PSU	N1-C2-N3	4.52	120.25	115.13
2	C	13	PSU	N1-C2-N3	4.50	120.23	115.13
48	w	1174	PSU	N1-C2-N3	4.50	120.23	115.13
48	w	36	PSU	C4-N3-C2	-4.49	119.87	126.34
3	D	4420	PSU	N1-C2-N3	4.49	120.22	115.13
48	w	814	PSU	N1-C2-N3	4.49	120.22	115.13
48	w	119	PSU	C4-N3-C2	-4.48	119.88	126.34
48	w	34	PSU	N1-C2-N3	4.48	120.20	115.13
48	w	572	PSU	N1-C2-N3	4.48	120.20	115.13
48	w	119	PSU	N1-C2-N3	4.47	120.20	115.13
48	w	210	PSU	N1-C2-N3	4.47	120.19	115.13
2	C	53	5MU	N3-C2-N1	4.44	120.78	114.89
48	w	93	PSU	N1-C2-N3	4.43	120.15	115.13
3	D	1792	PSU	N1-C2-N3	4.41	120.13	115.13
48	w	609	PSU	C4-N3-C2	-4.40	120.00	126.34
2	B	54	PSU	N1-C2-N3	4.40	120.11	115.13
48	w	218	PSU	N1-C2-N3	4.37	120.08	115.13
48	w	822	PSU	N1-C2-N3	4.37	120.08	115.13
48	w	822	PSU	C4-N3-C2	-4.37	120.05	126.34
2	B	53	5MU	C5M-C5-C4	4.35	123.56	118.77
48	w	1832	6MZ	C2-N1-C6	4.31	120.28	116.59
48	w	34	PSU	C4-N3-C2	-4.21	120.27	126.34
2	B	53	5MU	C5M-C5-C6	-4.16	117.29	122.85
3	D	3925	OMU	N3-C2-N1	4.16	120.41	114.89
2	B	53	5MU	N3-C2-N1	4.15	120.40	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2415	OMU	N3-C2-N1	4.12	120.35	114.89
2	C	53	5MU	C5M-C5-C6	-4.04	117.45	122.85
3	D	4306	OMU	N3-C2-N1	4.00	120.20	114.89
2	C	53	5MU	C5M-C5-C4	3.99	123.16	118.77
48	w	428	OMU	N3-C2-N1	3.97	120.16	114.89
3	D	4620	OMU	N3-C2-N1	3.97	120.16	114.89
3	D	2837	OMU	N3-C2-N1	3.97	120.16	114.89
3	D	4498	OMU	N3-C2-N1	3.94	120.12	114.89
3	D	4227	OMU	N3-C2-N1	3.91	120.08	114.89
3	D	4447	5MC	C5-C6-N1	-3.87	119.36	123.34
3	D	1773	OMU	N3-C2-N1	3.85	120.00	114.89
48	w	1326	OMU	N3-C2-N1	3.82	119.97	114.89
48	w	627	OMU	N3-C2-N1	3.80	119.94	114.89
48	w	1442	OMU	N3-C2-N1	3.80	119.94	114.89
48	w	799	OMU	N3-C2-N1	3.78	119.91	114.89
48	w	1804	OMU	N3-C2-N1	3.78	119.90	114.89
48	w	1288	OMU	N3-C2-N1	3.71	119.82	114.89
3	D	4392	OMG	C5-C6-N1	3.70	120.49	113.95
48	w	172	OMU	N3-C2-N1	3.70	119.80	114.89
48	w	121	OMU	N3-C2-N1	3.69	119.79	114.89
3	D	2415	OMU	C5-C4-N3	3.68	120.35	114.84
48	w	683	OMG	C5-C6-N1	3.65	120.39	113.95
3	D	4228	OMG	C5-C6-N1	3.64	120.37	113.95
48	w	436	OMG	C5-C6-N1	3.62	120.34	113.95
3	D	4370	OMG	C5-C6-N1	3.61	120.32	113.95
3	D	2837	OMU	C5-C4-N3	3.60	120.23	114.84
3	D	3627	OMG	C5-C6-N1	3.60	120.30	113.95
48	w	1337	4AC	O7-C7-N4	3.60	127.64	121.82
3	D	4498	OMU	C5-C4-N3	3.57	120.19	114.84
3	D	1625	OMG	C5-C6-N1	3.56	120.24	113.95
3	D	2424	OMG	C5-C6-N1	3.56	120.24	113.95
48	w	601	OMG	C5-C6-N1	3.55	120.22	113.95
3	D	1316	OMG	C5-C6-N1	3.54	120.21	113.95
3	D	1522	OMG	C5-C6-N1	3.54	120.20	113.95
3	D	3744	OMG	C5-C6-N1	3.54	120.20	113.95
3	D	2364	OMG	C5-C6-N1	3.54	120.20	113.95
3	D	4637	OMG	C5-C6-N1	3.53	120.19	113.95
2	B	6	2MG	C5-C6-N1	3.52	120.17	113.95
3	D	4499	OMG	C5-C6-N1	3.52	120.16	113.95
3	D	3925	OMU	C5-C4-N3	3.51	120.09	114.84
3	D	4494	OMG	C5-C6-N1	3.51	120.14	113.95
5	F	75	OMG	C5-C6-N1	3.50	120.13	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4227	OMU	C5-C4-N3	3.49	120.06	114.84
3	D	3899	OMG	C5-C6-N1	3.48	120.10	113.95
48	w	116	OMU	C5-C4-N3	3.48	120.04	114.84
48	w	1804	OMU	C5-C4-N3	3.47	120.04	114.84
3	D	4196	OMG	C5-C6-N1	3.47	120.08	113.95
48	w	1490	OMG	C5-C6-N1	3.47	120.08	113.95
3	D	3782	5MC	C5-C6-N1	-3.47	119.77	123.34
3	D	3792	OMG	C5-C6-N1	3.47	120.07	113.95
2	C	47	5MC	C5-C6-N1	-3.46	119.78	123.34
3	D	3944	OMG	C5-C6-N1	3.46	120.07	113.95
2	C	6	2MG	C5-C6-N1	3.46	120.06	113.95
48	w	644	OMG	C5-C6-N1	3.46	120.06	113.95
48	w	116	OMU	N3-C2-N1	3.45	119.48	114.89
48	w	1328	OMG	C5-C6-N1	3.44	120.03	113.95
3	D	4306	OMU	C5-C4-N3	3.43	119.98	114.84
2	B	47	5MC	C5-C6-N1	-3.43	119.81	123.34
3	D	4620	OMU	C5-C4-N3	3.43	119.97	114.84
48	w	1842	4AC	O7-C7-N4	3.41	127.33	121.82
3	D	4623	OMG	C5-C6-N1	3.40	119.95	113.95
3	D	4618	OMG	C5-C6-N1	3.39	119.95	113.95
2	B	38	5MC	C5-C6-N1	-3.39	119.85	123.34
48	w	509	OMG	C5-C6-N1	3.38	119.92	113.95
3	D	1760	OMG	C5-C6-N1	3.36	119.89	113.95
48	w	172	OMU	C5-C4-N3	3.35	119.85	114.84
48	w	1442	OMU	C5-C4-N3	3.34	119.83	114.84
2	B	48	5MC	C5-C6-N1	-3.33	119.91	123.34
48	w	627	OMU	C5-C4-N3	3.32	119.80	114.84
48	w	799	OMU	C5-C4-N3	3.30	119.77	114.84
2	C	38	5MC	C5-C6-N1	-3.29	119.95	123.34
48	w	1288	OMU	C5-C4-N3	3.28	119.75	114.84
48	w	1326	OMU	C5-C4-N3	3.26	119.72	114.84
48	w	121	OMU	C5-C4-N3	3.25	119.70	114.84
3	D	1773	OMU	C5-C4-N3	3.22	119.65	114.84
48	w	428	OMU	C5-C4-N3	3.20	119.63	114.84
2	C	48	5MC	C5-C6-N1	-3.16	120.09	123.34
48	w	436	OMG	C2-N1-C6	-3.13	119.34	125.10
48	w	683	OMG	C2-N1-C6	-3.12	119.36	125.10
3	D	1625	OMG	C2-N1-C6	-3.12	119.36	125.10
3	D	4392	OMG	C2-N1-C6	-3.11	119.36	125.10
48	w	1639	G7M	C2-N1-C6	-3.10	119.38	125.10
2	B	34	56B	C2-N1-C6	-3.09	119.40	125.10
3	D	2424	OMG	C2-N1-C6	-3.09	119.42	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4196	OMG	C2-N1-C6	-3.08	119.42	125.10
48	w	644	OMG	C2-N1-C6	-3.07	119.45	125.10
3	D	3744	OMG	C2-N1-C6	-3.06	119.46	125.10
3	D	3792	OMG	C2-N1-C6	-3.05	119.48	125.10
3	D	2364	OMG	C2-N1-C6	-3.05	119.48	125.10
3	D	4499	OMG	C2-N1-C6	-3.04	119.49	125.10
3	D	4637	OMG	C2-N1-C6	-3.04	119.50	125.10
48	w	1328	OMG	C2-N1-C6	-3.04	119.51	125.10
2	C	34	56B	C2-N1-C6	-3.03	119.51	125.10
3	D	1316	OMG	C2-N1-C6	-3.03	119.52	125.10
3	D	3627	OMG	C2-N1-C6	-3.03	119.52	125.10
48	w	116	OMU	O4-C4-C5	-3.02	119.85	125.16
3	D	4228	OMG	C2-N1-C6	-3.01	119.55	125.10
3	D	4494	OMG	C2-N1-C6	-3.00	119.58	125.10
3	D	3944	OMG	C2-N1-C6	-2.99	119.59	125.10
5	F	75	OMG	C2-N1-C6	-2.99	119.60	125.10
48	w	1490	OMG	C2-N1-C6	-2.97	119.62	125.10
48	w	509	OMG	C2-N1-C6	-2.96	119.66	125.10
48	w	601	OMG	C2-N1-C6	-2.95	119.66	125.10
48	w	1804	OMU	O4-C4-C5	-2.95	119.97	125.16
48	w	1851	MA6	N1-C6-N6	-2.95	113.96	117.06
3	D	4370	OMG	C2-N1-C6	-2.94	119.68	125.10
3	D	1522	OMG	C2-N1-C6	-2.94	119.68	125.10
3	D	4576	PSU	O2-C2-N1	-2.94	119.56	122.79
3	D	4500	PSU	O2-C2-N1	-2.93	119.57	122.79
3	D	2837	OMU	O4-C4-C5	-2.92	120.02	125.16
3	D	4618	OMG	C2-N1-C6	-2.92	119.73	125.10
3	D	1683	PSU	O2-C2-N1	-2.92	119.58	122.79
3	D	3920	PSU	O2-C2-N1	-2.91	119.59	122.79
3	D	2415	OMU	O4-C4-C5	-2.89	120.08	125.16
48	w	644	OMG	C8-N7-C5	2.87	108.47	102.99
3	D	3899	OMG	C2-N1-C6	-2.87	119.81	125.10
3	D	3695	PSU	O2-C2-N1	-2.87	119.63	122.79
48	w	172	OMU	O4-C4-C5	-2.86	120.12	125.16
3	D	4623	OMG	C2-N1-C6	-2.86	119.83	125.10
2	B	6	2MG	C8-N7-C5	2.86	108.44	102.99
3	D	4306	OMU	O4-C4-C5	-2.86	120.14	125.16
48	w	1442	OMU	O4-C4-C5	-2.86	120.14	125.16
3	D	3925	OMU	O4-C4-C5	-2.85	120.14	125.16
48	w	1004	PSU	O2-C2-N1	-2.85	119.65	122.79
48	w	109	PSU	O2-C2-N1	-2.84	119.66	122.79
48	w	436	OMG	C8-N7-C5	2.83	108.39	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4227	OMU	O4-C4-C5	-2.83	120.18	125.16
48	w	36	PSU	O2-C2-N1	-2.83	119.68	122.79
48	w	627	OMU	O4-C4-C5	-2.83	120.19	125.16
48	w	1328	OMG	C8-N7-C5	2.82	108.37	102.99
3	D	4498	OMU	O4-C4-C5	-2.82	120.20	125.16
48	w	119	PSU	O2-C2-N1	-2.82	119.69	122.79
48	w	1046	PSU	O2-C2-N1	-2.82	119.69	122.79
48	w	1326	OMU	O4-C4-C5	-2.81	120.22	125.16
2	C	6	2MG	C8-N7-C5	2.81	108.34	102.99
48	w	1288	OMU	O4-C4-C5	-2.81	120.22	125.16
3	D	1860	PSU	O2-C2-N1	-2.80	119.70	122.79
3	D	1683	PSU	C6-N1-C2	-2.80	119.82	122.68
3	D	4620	OMU	O4-C4-C5	-2.79	120.25	125.16
3	D	4228	OMG	C8-N7-C5	2.79	108.30	102.99
3	D	3768	PSU	O2-C2-N1	-2.79	119.72	122.79
3	D	3762	PSU	O2-C2-N1	-2.78	119.72	122.79
3	D	4623	OMG	C8-N7-C5	2.77	108.27	102.99
3	D	1534	A2M	C3'-C2'-C1'	-2.77	97.68	102.89
3	D	4431	PSU	O2-C2-N1	-2.77	119.74	122.79
48	w	822	PSU	O2-C2-N1	-2.77	119.74	122.79
48	w	683	OMG	C8-N7-C5	2.76	108.25	102.99
3	D	5010	PSU	O2-C2-N1	-2.76	119.75	122.79
48	w	799	OMU	O4-C4-C5	-2.76	120.31	125.16
3	D	1760	OMG	C8-N7-C5	2.76	108.24	102.99
48	w	601	OMG	C8-N7-C5	2.75	108.24	102.99
5	F	75	OMG	C8-N7-C5	2.74	108.22	102.99
3	D	1760	OMG	C2-N1-C6	-2.74	120.05	125.10
3	D	1536	PSU	O2-C2-N1	-2.74	119.77	122.79
3	D	4579	PSU	O2-C2-N1	-2.74	119.77	122.79
3	D	1316	OMG	C8-N7-C5	2.74	108.21	102.99
3	D	4499	OMG	C8-N7-C5	2.74	108.21	102.99
3	D	1773	OMU	O4-C4-C5	-2.74	120.35	125.16
2	B	13	PSU	O2-C2-N1	-2.73	119.78	122.79
48	w	609	PSU	O2-C2-N1	-2.73	119.78	122.79
3	D	3944	OMG	C8-N7-C5	2.73	108.20	102.99
3	D	1534	A2M	O2'-C2'-C1'	2.73	114.51	109.09
3	D	4494	OMG	C8-N7-C5	2.73	108.19	102.99
48	w	1177	PSU	O2-C2-N1	-2.73	119.79	122.79
3	D	4637	OMG	C8-N7-C5	2.72	108.18	102.99
48	w	801	PSU	O2-C2-N1	-2.72	119.79	122.79
3	D	4370	OMG	C8-N7-C5	2.72	108.17	102.99
3	D	3627	OMG	C8-N7-C5	2.72	108.17	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4618	OMG	C8-N7-C5	2.72	108.17	102.99
3	D	1522	OMG	C8-N7-C5	2.72	108.17	102.99
48	w	509	OMG	C8-N7-C5	2.72	108.17	102.99
3	D	1625	OMG	C8-N7-C5	2.71	108.16	102.99
3	D	3899	OMG	C8-N7-C5	2.71	108.16	102.99
48	w	121	OMU	O4-C4-C5	-2.71	120.40	125.16
48	w	966	PSU	O2-C2-N1	-2.71	119.81	122.79
3	D	3744	OMG	C8-N7-C5	2.70	108.14	102.99
3	D	3734	PSU	O2-C2-N1	-2.70	119.82	122.79
3	D	1744	PSU	O2-C2-N1	-2.70	119.82	122.79
3	D	4442	PSU	O2-C2-N1	-2.70	119.82	122.79
3	D	4392	OMG	C8-N7-C5	2.69	108.12	102.99
48	w	1238	PSU	O2-C2-N1	-2.69	119.83	122.79
48	w	686	PSU	O2-C2-N1	-2.69	119.83	122.79
3	D	2632	PSU	O2-C2-N1	-2.69	119.83	122.79
3	D	4403	PSU	O2-C2-N1	-2.69	119.83	122.79
48	w	866	PSU	O2-C2-N1	-2.69	119.83	122.79
48	w	428	OMU	O4-C4-C5	-2.68	120.45	125.16
48	w	649	PSU	O2-C2-N1	-2.68	119.84	122.79
3	D	4312	PSU	O2-C2-N1	-2.67	119.85	122.79
48	w	1367	PSU	O2-C2-N1	-2.67	119.86	122.79
3	D	3715	PSU	O2-C2-N1	-2.66	119.87	122.79
3	D	2364	OMG	C8-N7-C5	2.66	108.05	102.99
3	D	2424	OMG	C8-N7-C5	2.65	108.04	102.99
3	D	4457	PSU	O2-C2-N1	-2.65	119.87	122.79
48	w	651	PSU	O2-C2-N1	-2.65	119.88	122.79
48	w	406	PSU	O2-C2-N1	-2.64	119.89	122.79
48	w	1326	OMU	C1'-N1-C2	2.64	122.35	117.57
3	D	3760	A2M	C3'-C2'-C1'	-2.64	97.93	102.89
48	w	1490	OMG	C8-N7-C5	2.63	108.00	102.99
3	D	1862	PSU	O2-C2-N1	-2.63	119.90	122.79
48	w	210	PSU	O2-C2-N1	-2.62	119.91	122.79
48	w	1692	PSU	O2-C2-N1	-2.62	119.91	122.79
3	D	4353	PSU	O2-C2-N1	-2.62	119.91	122.79
3	D	3792	OMG	C8-N7-C5	2.61	107.97	102.99
3	D	4423	PSU	O2-C2-N1	-2.61	119.91	122.79
48	w	1643	PSU	O2-C2-N1	-2.61	119.91	122.79
48	w	36	PSU	C6-C5-C4	2.61	120.02	118.20
3	D	3764	PSU	O2-C2-N1	-2.61	119.92	122.79
2	C	54	PSU	O2-C2-N1	-2.60	119.92	122.79
3	D	1782	PSU	O2-C2-N1	-2.60	119.92	122.79
3	D	4972	PSU	O2-C2-N1	-2.59	119.94	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	1625	PSU	O2-C2-N1	-2.59	119.94	122.79
48	w	1347	PSU	O2-C2-N1	-2.58	119.95	122.79
3	D	4299	PSU	O2-C2-N1	-2.58	119.95	122.79
3	D	4361	PSU	O2-C2-N1	-2.58	119.95	122.79
3	D	4500	PSU	C6-N1-C2	-2.58	120.05	122.68
3	D	4196	OMG	C8-N7-C5	2.58	107.90	102.99
48	w	1445	PSU	O2-C2-N1	-2.57	119.96	122.79
3	D	3851	PSU	O2-C2-N1	-2.57	119.96	122.79
48	w	1232	PSU	O2-C2-N1	-2.57	119.96	122.79
48	w	1045	PSU	O2-C2-N1	-2.57	119.96	122.79
3	D	4293	PSU	O2-C2-N1	-2.56	119.97	122.79
48	w	1383	A2M	C3'-C2'-C1'	-2.56	98.08	102.89
48	w	1244	PSU	O2-C2-N1	-2.56	119.97	122.79
2	B	53	5MU	O4-C4-N3	-2.56	115.21	120.12
3	D	3770	PSU	O2-C2-N1	-2.56	119.98	122.79
48	w	36	PSU	C6-N1-C2	-2.56	120.07	122.68
3	D	4689	PSU	O2-C2-N1	-2.55	119.98	122.79
48	w	863	PSU	O2-C2-N1	-2.55	119.98	122.79
3	D	4220	6MZ	C4-C5-N7	-2.55	106.74	109.40
3	D	1860	PSU	C6-N1-C2	-2.54	120.08	122.68
48	w	681	PSU	O2-C2-N1	-2.54	120.00	122.79
3	D	1781	PSU	O2-C2-N1	-2.54	120.00	122.79
2	C	13	PSU	O2-C2-N1	-2.53	120.00	122.79
3	D	3730	PSU	O2-C2-N1	-2.53	120.01	122.79
3	D	4532	PSU	O2-C2-N1	-2.53	120.01	122.79
3	D	1677	PSU	O2-C2-N1	-2.52	120.01	122.79
48	w	105	PSU	O2-C2-N1	-2.51	120.03	122.79
2	C	53	5MU	O4-C4-N3	-2.51	115.31	120.12
3	D	4521	PSU	O2-C2-N1	-2.51	120.03	122.79
48	w	815	PSU	O2-C2-N1	-2.50	120.03	122.79
48	w	1081	PSU	O2-C2-N1	-2.50	120.04	122.79
3	D	4628	PSU	O2-C2-N1	-2.49	120.04	122.79
48	w	609	PSU	C6-N1-C2	-2.49	120.13	122.68
3	D	4392	OMG	O6-C6-C5	-2.49	119.51	124.37
3	D	4579	PSU	C6-N1-C2	-2.49	120.14	122.68
3	D	4296	PSU	O2-C2-N1	-2.48	120.06	122.79
3	D	2837	OMU	O2-C2-N1	-2.48	119.50	122.79
3	D	4552	PSU	O2-C2-N1	-2.47	120.07	122.79
48	w	1337	4AC	CM7-C7-N4	-2.47	111.02	115.29
3	D	4420	PSU	O2-C2-N1	-2.47	120.07	122.79
2	B	54	PSU	O2-C2-N1	-2.47	120.08	122.79
48	w	218	PSU	O2-C2-N1	-2.46	120.08	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	PSU	C6-N1-C2	-2.46	120.17	122.68
3	D	2424	OMG	O6-C6-C5	-2.45	119.58	124.37
48	w	1004	PSU	C6-N1-C2	-2.45	120.17	122.68
3	D	3770	PSU	C6-N1-C2	-2.45	120.18	122.68
48	w	109	PSU	C6-N1-C2	-2.44	120.18	122.68
48	w	1643	PSU	C6-N1-C2	-2.44	120.18	122.68
48	w	34	PSU	O2-C2-N1	-2.44	120.11	122.79
3	D	4628	PSU	C6-N1-C2	-2.43	120.19	122.68
3	D	4299	PSU	C6-N1-C2	-2.43	120.20	122.68
3	D	3639	PSU	O2-C2-N1	-2.43	120.12	122.79
48	w	572	PSU	O2-C2-N1	-2.43	120.12	122.79
3	D	4423	PSU	C6-N1-C2	-2.42	120.21	122.68
3	D	4689	PSU	C6-N1-C2	-2.42	120.21	122.68
3	D	3762	PSU	C6-N1-C2	-2.41	120.22	122.68
3	D	4552	PSU	C6-N1-C2	-2.41	120.22	122.68
3	D	1625	OMG	O6-C6-C5	-2.41	119.67	124.37
2	C	53	5MU	O2-C2-N1	-2.41	119.59	122.79
3	D	4228	OMG	O6-C6-C5	-2.41	119.67	124.37
48	w	34	PSU	C6-N1-C2	-2.40	120.23	122.68
2	C	34	56B	C9-C7-C8	-2.40	124.30	127.67
3	D	4403	PSU	C6-N1-C2	-2.40	120.23	122.68
3	D	2508	PSU	O2-C2-N1	-2.39	120.16	122.79
3	D	3744	OMG	O6-C6-C5	-2.39	119.70	124.37
3	D	2364	OMG	O6-C6-C5	-2.39	119.71	124.37
3	D	3758	PSU	O2-C2-N1	-2.38	120.17	122.79
3	D	4293	PSU	C6-N1-C2	-2.38	120.25	122.68
3	D	2415	OMU	O3'-C3'-C2'	2.38	117.92	111.17
3	D	4620	OMU	O2-C2-N1	-2.38	119.63	122.79
48	w	93	PSU	O2-C2-N1	-2.37	120.18	122.79
48	w	1046	PSU	C6-N1-C2	-2.37	120.26	122.68
3	D	4532	PSU	C6-N1-C2	-2.37	120.26	122.68
3	D	3627	OMG	O6-C6-C5	-2.37	119.74	124.37
48	w	1842	4AC	C5-C4-N4	-2.37	118.81	122.92
3	D	3792	OMG	O6-C6-C5	-2.37	119.75	124.37
48	w	686	PSU	C6-N1-C2	-2.36	120.27	122.68
3	D	3764	PSU	C6-N1-C2	-2.36	120.27	122.68
3	D	4296	PSU	C6-N1-C2	-2.36	120.27	122.68
3	D	4361	PSU	C6-N1-C2	-2.36	120.27	122.68
48	w	436	OMG	O6-C6-C5	-2.36	119.77	124.37
48	w	1850	MA6	N1-C6-N6	-2.35	114.58	117.06
3	D	4972	PSU	C6-N1-C2	-2.35	120.28	122.68
48	w	1232	PSU	C6-N1-C2	-2.35	120.28	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3768	PSU	C6-N1-C2	-2.35	120.28	122.68
48	w	651	PSU	C6-C5-C4	2.35	119.84	118.20
3	D	1744	PSU	C6-N1-C2	-2.35	120.28	122.68
48	w	822	PSU	O4'-C1'-C2'	2.35	108.45	105.14
3	D	3734	PSU	C6-C5-C4	2.35	119.84	118.20
3	D	4431	PSU	C6-N1-C2	-2.35	120.28	122.68
3	D	4499	OMG	O6-C6-C5	-2.35	119.79	124.37
3	D	1316	OMG	O6-C6-C5	-2.34	119.79	124.37
48	w	863	PSU	C6-N1-C2	-2.34	120.29	122.68
48	w	1174	PSU	O2-C2-N1	-2.34	120.21	122.79
3	D	3734	PSU	C6-N1-C2	-2.34	120.29	122.68
48	w	1056	PSU	O2-C2-N1	-2.34	120.22	122.79
3	D	3851	PSU	C6-N1-C2	-2.33	120.30	122.68
3	D	4442	PSU	C6-N1-C2	-2.33	120.30	122.68
48	w	509	OMG	O6-C6-C5	-2.33	119.83	124.37
3	D	1871	A2M	C3'-C2'-C1'	-2.32	98.52	102.89
3	D	4471	PSU	O2-C2-N1	-2.32	120.23	122.79
48	w	1842	4AC	C4-N3-C2	-2.31	116.97	120.12
3	D	3639	PSU	C6-N1-C2	-2.31	120.32	122.68
3	D	5001	PSU	O2-C2-N1	-2.31	120.25	122.79
48	w	814	PSU	O2-C2-N1	-2.31	120.25	122.79
48	w	105	PSU	C6-N1-C2	-2.31	120.32	122.68
3	D	3695	PSU	C6-N1-C2	-2.31	120.33	122.68
48	w	1238	PSU	C6-N1-C2	-2.31	120.33	122.68
3	D	5010	PSU	C6-N1-C2	-2.30	120.33	122.68
3	D	3853	PSU	O2-C2-N1	-2.30	120.26	122.79
48	w	649	PSU	C6-N1-C2	-2.30	120.33	122.68
3	D	3853	PSU	C6-N1-C2	-2.30	120.33	122.68
48	w	601	OMG	O6-C6-C5	-2.30	119.88	124.37
3	D	4306	OMU	O2-C2-N1	-2.30	119.73	122.79
48	w	119	PSU	C6-N1-C2	-2.29	120.34	122.68
3	D	1792	PSU	O2-C2-N1	-2.29	120.27	122.79
48	w	406	PSU	C6-C5-C4	2.29	119.80	118.20
3	D	1862	PSU	C6-N1-C2	-2.29	120.34	122.68
3	D	3637	PSU	O2-C2-N1	-2.29	120.27	122.79
5	F	75	OMG	O6-C6-C5	-2.29	119.91	124.37
3	D	4637	OMG	O6-C6-C5	-2.29	119.91	124.37
3	D	1536	PSU	C6-N1-C2	-2.28	120.35	122.68
48	w	1625	PSU	C6-N1-C2	-2.28	120.35	122.68
3	D	3715	PSU	C6-N1-C2	-2.28	120.35	122.68
48	w	815	PSU	C6-C5-C4	2.28	119.79	118.20
48	w	1367	PSU	C6-C5-C4	2.28	119.79	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4196	OMG	O6-C6-C5	-2.28	119.93	124.37
2	B	6	2MG	O6-C6-C5	-2.27	119.94	124.37
48	w	683	OMG	O6-C6-C5	-2.27	119.94	124.37
3	D	4353	PSU	C6-N1-C2	-2.26	120.37	122.68
48	w	966	PSU	C6-N1-C2	-2.26	120.37	122.68
3	D	4457	PSU	C6-N1-C2	-2.26	120.37	122.68
3	D	4494	OMG	O6-C6-C5	-2.26	119.96	124.37
2	C	6	2MG	O6-C6-C5	-2.25	119.97	124.37
48	w	822	PSU	C6-N1-C2	-2.25	120.38	122.68
3	D	1781	PSU	C6-N1-C2	-2.25	120.38	122.68
3	D	2632	PSU	C6-N1-C2	-2.25	120.38	122.68
48	w	1490	OMG	O6-C6-C5	-2.25	119.98	124.37
3	D	3758	PSU	C6-N1-C2	-2.23	120.40	122.68
48	w	1851	MA6	C4-C5-N7	-2.23	107.07	109.40
3	D	3944	OMG	O6-C6-C5	-2.23	120.01	124.37
48	w	681	PSU	C6-N1-C2	-2.23	120.40	122.68
48	w	1045	PSU	C6-C5-C4	2.23	119.76	118.20
48	w	681	PSU	C6-C5-C4	2.23	119.75	118.20
3	D	3785	A2M	C2-N1-C6	-2.23	114.95	118.75
48	w	649	PSU	C6-C5-C4	2.23	119.75	118.20
3	D	4370	OMG	O6-C6-C5	-2.22	120.03	124.37
3	D	3637	PSU	C6-N1-C2	-2.22	120.41	122.68
48	w	801	PSU	C6-N1-C2	-2.22	120.41	122.68
3	D	4312	PSU	C6-N1-C2	-2.22	120.42	122.68
3	D	2508	PSU	C6-N1-C2	-2.22	120.42	122.68
3	D	1534	A2M	C2-N1-C6	-2.21	114.97	118.75
3	D	4576	PSU	C6-N1-C2	-2.21	120.43	122.68
3	D	4471	PSU	C6-N1-C2	-2.20	120.43	122.68
2	B	13	PSU	C6-C5-C4	2.20	119.74	118.20
3	D	3920	PSU	C6-N1-C2	-2.20	120.43	122.68
48	w	1337	4AC	C5-C4-N4	-2.20	119.10	122.92
48	w	1174	PSU	C6-N1-C2	-2.20	120.43	122.68
48	w	1328	OMG	O6-C6-C5	-2.20	120.08	124.37
2	C	54	PSU	C6-N1-C2	-2.20	120.44	122.68
3	D	4420	PSU	C6-N1-C2	-2.19	120.44	122.68
3	D	4521	PSU	C6-N1-C2	-2.19	120.44	122.68
48	w	1445	PSU	C6-N1-C2	-2.19	120.44	122.68
48	w	1692	PSU	C6-N1-C2	-2.19	120.44	122.68
48	w	1056	PSU	C6-N1-C2	-2.19	120.44	122.68
48	w	1081	PSU	O4'-C1'-C2'	2.19	108.23	105.14
2	C	13	PSU	C6-N1-C2	-2.19	120.44	122.68
2	B	34	56B	C9-C7-C8	-2.19	124.60	127.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1782	PSU	C6-N1-C2	-2.19	120.45	122.68
48	w	1248	B8N	C32-C33-C34	-2.19	105.10	110.30
3	D	3782	5MC	CM5-C5-C6	-2.18	119.94	122.85
3	D	4623	OMG	O6-C6-C5	-2.17	120.12	124.37
48	w	1347	PSU	C6-N1-C2	-2.17	120.46	122.68
3	D	3925	OMU	O2-C2-N1	-2.17	119.90	122.79
48	w	1045	PSU	C6-N1-C2	-2.17	120.46	122.68
3	D	4523	A2M	C2-N1-C6	-2.17	115.05	118.75
3	D	4420	PSU	O4'-C1'-C2'	2.17	108.20	105.14
3	D	3818	UY1	O4-C4-N3	-2.16	115.97	120.12
48	w	1177	PSU	C6-N1-C2	-2.16	120.47	122.68
3	D	2815	A2M	C2-N1-C6	-2.16	115.06	118.75
3	D	4498	OMU	O2-C2-N1	-2.16	119.91	122.79
48	w	1367	PSU	C6-N1-C2	-2.16	120.47	122.68
3	D	4523	A2M	C3'-C2'-C1'	-2.16	98.83	102.89
3	D	1862	PSU	C6-C5-C4	2.16	119.71	118.20
48	w	644	OMG	O6-C6-C5	-2.16	120.16	124.37
48	w	406	PSU	C6-N1-C2	-2.15	120.48	122.68
3	D	3899	OMG	O6-C6-C5	-2.15	120.17	124.37
48	w	1639	G7M	O3'-C3'-C2'	2.14	118.76	111.82
48	w	1850	MA6	C4-C5-N7	-2.14	107.17	109.40
3	D	2415	OMU	O2-C2-N1	-2.14	119.94	122.79
48	w	1842	4AC	CM7-C7-N4	-2.14	111.60	115.29
3	D	3730	PSU	C6-N1-C2	-2.14	120.50	122.68
48	w	1678	A2M	C2-N1-C6	-2.13	115.11	118.75
3	D	2787	A2M	C2-N1-C6	-2.13	115.11	118.75
48	w	218	PSU	C6-N1-C2	-2.13	120.50	122.68
48	w	159	A2M	C2-N1-C6	-2.13	115.11	118.75
3	D	1522	OMG	O6-C6-C5	-2.13	120.22	124.37
48	w	1248	B8N	O4'-C1'-C2'	2.12	108.14	105.14
48	w	210	PSU	C6-N1-C2	-2.12	120.51	122.68
48	w	651	PSU	C6-N1-C2	-2.12	120.52	122.68
3	D	2401	A2M	C2-N1-C6	-2.12	115.13	118.75
2	B	48	5MC	CM5-C5-C6	-2.12	120.02	122.85
3	D	2363	A2M	C2-N1-C6	-2.12	115.13	118.75
48	w	1442	OMU	O2-C2-N1	-2.12	119.97	122.79
3	D	4618	OMG	O6-C6-C5	-2.11	120.24	124.37
3	D	3715	PSU	C6-C5-C4	2.11	119.67	118.20
48	w	1238	PSU	C6-C5-C4	2.11	119.67	118.20
3	D	1524	A2M	C2-N1-C6	-2.11	115.15	118.75
3	D	5001	PSU	C6-N1-C2	-2.11	120.53	122.68
48	w	512	A2M	C3'-C2'-C1'	-2.11	98.93	102.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1760	OMG	O6-C6-C5	-2.11	120.25	124.37
48	w	866	PSU	C6-N1-C2	-2.11	120.53	122.68
48	w	99	A2M	C2-N1-C6	-2.10	115.15	118.75
2	B	54	PSU	C6-N1-C2	-2.10	120.53	122.68
3	D	3724	A2M	C2-N1-C6	-2.10	115.17	118.75
48	w	966	PSU	C6-C5-C4	2.09	119.66	118.20
3	D	3825	A2M	C2-N1-C6	-2.09	115.17	118.75
3	D	3718	A2M	C2-N1-C6	-2.09	115.17	118.75
48	w	1383	A2M	C2-N1-C6	-2.09	115.18	118.75
48	w	484	A2M	C2-N1-C6	-2.09	115.19	118.75
3	D	4442	PSU	C6-C5-C4	2.08	119.65	118.20
3	D	400	A2M	C2-N1-C6	-2.08	115.20	118.75
3	D	3851	PSU	C6-C5-C4	2.08	119.65	118.20
3	D	1326	A2M	C2-N1-C6	-2.08	115.20	118.75
48	w	1337	4AC	C4-N3-C2	-2.08	117.29	120.12
48	w	428	OMU	O2-C2-N1	-2.07	120.03	122.79
48	w	590	A2M	C2-N1-C6	-2.07	115.21	118.75
3	D	398	A2M	C2-N1-C6	-2.07	115.21	118.75
3	D	4442	PSU	O4'-C1'-C2'	2.07	108.06	105.14
48	w	815	PSU	C6-N1-C2	-2.06	120.57	122.68
48	w	1244	PSU	C6-N1-C2	-2.06	120.57	122.68
48	w	1643	PSU	C6-C5-C4	2.06	119.64	118.20
2	B	47	5MC	CM5-C5-C6	-2.06	120.10	122.85
48	w	210	PSU	C6-C5-C4	2.05	119.63	118.20
2	B	38	5MC	CM5-C5-C6	-2.05	120.11	122.85
3	D	4530	UR3	C6-N1-C2	-2.05	119.95	121.79
2	C	38	5MC	CM5-C5-C6	-2.04	120.12	122.85
48	w	166	A2M	C2-N1-C6	-2.04	115.26	118.75
3	D	3760	A2M	C2-N1-C6	-2.04	115.26	118.75
48	w	1337	4AC	C5-C4-N3	2.04	125.88	122.59
48	w	627	OMU	O2-C2-N1	-2.04	120.08	122.79
48	w	668	A2M	C2-N1-C6	-2.04	115.27	118.75
3	D	1677	PSU	C6-N1-C2	-2.04	120.60	122.68
2	C	47	5MC	CM5-C5-C6	-2.03	120.13	122.85
48	w	1326	OMU	O2'-C2'-C1'	2.03	113.04	109.08
3	D	4521	PSU	O4'-C1'-C2'	2.03	108.01	105.14
48	w	863	PSU	C6-C5-C4	2.03	119.61	118.20
48	w	576	A2M	C2-N1-C6	-2.02	115.29	118.75
2	C	48	5MC	CM5-C5-C6	-2.02	120.15	122.85
48	w	105	PSU	C6-C5-C4	2.02	119.61	118.20
3	D	3730	PSU	C6-C5-C4	2.01	119.60	118.20
3	D	4403	PSU	C6-C5-C4	2.01	119.60	118.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	w	814	PSU	C6-N1-C2	-2.01	120.63	122.68
48	w	172	OMU	O2-C2-N1	-2.00	120.12	122.79
3	D	1683	PSU	C6-C5-C4	2.00	119.60	118.20
3	D	5010	PSU	C6-C5-C4	2.00	119.60	118.20
48	w	1445	PSU	C6-C5-C4	2.00	119.60	118.20

There are no chirality outliers.

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	34	56B	C14-C10-N10-C9
2	C	34	56B	C11-C10-N10-C9
2	C	34	56B	C14-C10-N10-C9
2	B	47	5MC	O4'-C4'-C5'-O5'
2	B	47	5MC	C3'-C4'-C5'-O5'
2	B	48	5MC	O4'-C4'-C5'-O5'
2	C	48	5MC	O4'-C4'-C5'-O5'
2	B	53	5MU	O4'-C4'-C5'-O5'
3	D	398	A2M	C1'-C2'-O2'-CM'
3	D	1534	A2M	C1'-C2'-O2'-CM'
3	D	1677	PSU	C2'-C1'-C5-C6
3	D	1760	OMG	C3'-C4'-C5'-O5'
3	D	1773	OMU	C1'-C2'-O2'-CM2
3	D	2415	OMU	C1'-C2'-O2'-CM2
3	D	2415	OMU	C3'-C4'-C5'-O5'
3	D	2415	OMU	O4'-C4'-C5'-O5'
3	D	2424	OMG	O4'-C4'-C5'-O5'
3	D	2424	OMG	C3'-C4'-C5'-O5'
3	D	2815	A2M	O4'-C4'-C5'-O5'
3	D	2815	A2M	C3'-C4'-C5'-O5'
3	D	3785	A2M	O4'-C4'-C5'-O5'
3	D	3944	OMG	O4'-C4'-C5'-O5'
3	D	3944	OMG	C3'-C4'-C5'-O5'
3	D	4196	OMG	C1'-C2'-O2'-CM2
3	D	4227	OMU	C1'-C2'-O2'-CM2
3	D	4500	PSU	C3'-C4'-C5'-O5'
3	D	4500	PSU	O4'-C4'-C5'-O5'
3	D	4637	OMG	C1'-C2'-O2'-CM2
48	w	34	PSU	C3'-C4'-C5'-O5'
48	w	116	OMU	O4'-C4'-C5'-O5'
48	w	159	A2M	O4'-C4'-C5'-O5'
48	w	159	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
48	w	166	A2M	O4'-C4'-C5'-O5'
48	w	166	A2M	C3'-C4'-C5'-O5'
48	w	174	OMC	C1'-C2'-O2'-CM2
48	w	428	OMU	C2'-C1'-N1-C2
48	w	428	OMU	C2'-C1'-N1-C6
48	w	428	OMU	C1'-C2'-O2'-CM2
48	w	468	A2M	O4'-C4'-C5'-O5'
48	w	468	A2M	C3'-C4'-C5'-O5'
48	w	512	A2M	C3'-C4'-C5'-O5'
48	w	576	A2M	C3'-C4'-C5'-O5'
48	w	627	OMU	C1'-C2'-O2'-CM2
48	w	644	OMG	C3'-C4'-C5'-O5'
48	w	668	A2M	O4'-C4'-C5'-O5'
48	w	668	A2M	C1'-C2'-O2'-CM'
48	w	799	OMU	C1'-C2'-O2'-CM2
48	w	1248	B8N	C31-C32-C33-N34
48	w	1326	OMU	C1'-C2'-O2'-CM2
48	w	1442	OMU	C1'-C2'-O2'-CM2
48	w	1639	G7M	O4'-C4'-C5'-O5'
48	w	1678	A2M	C1'-C2'-O2'-CM'
48	w	1804	OMU	C1'-C2'-O2'-CM2
48	w	1832	6MZ	C5-C6-N6-C9
48	w	1832	6MZ	N1-C6-N6-C9
48	w	1851	MA6	O4'-C4'-C5'-O5'
3	D	3701	OMC	C2'-C1'-N1-C6
2	C	47	5MC	C3'-C4'-C5'-O5'
2	B	48	5MC	C3'-C4'-C5'-O5'
2	C	48	5MC	C3'-C4'-C5'-O5'
2	B	53	5MU	C3'-C4'-C5'-O5'
3	D	1534	A2M	O4'-C4'-C5'-O5'
3	D	3785	A2M	C3'-C4'-C5'-O5'
3	D	3818	UY1	C3'-C4'-C5'-O5'
3	D	3818	UY1	O4'-C4'-C5'-O5'
48	w	116	OMU	C3'-C4'-C5'-O5'
48	w	428	OMU	C3'-C4'-C5'-O5'
48	w	512	A2M	O4'-C4'-C5'-O5'
48	w	627	OMU	C3'-C4'-C5'-O5'
48	w	627	OMU	O4'-C4'-C5'-O5'
48	w	822	PSU	C3'-C4'-C5'-O5'
48	w	1238	PSU	C3'-C4'-C5'-O5'
48	w	1288	OMU	C3'-C4'-C5'-O5'
48	w	1851	MA6	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	34	56B	C7-C9-N10-C10
3	D	1760	OMG	O4'-C4'-C5'-O5'
3	D	2364	OMG	O4'-C4'-C5'-O5'
48	w	428	OMU	O4'-C4'-C5'-O5'
48	w	576	A2M	O4'-C4'-C5'-O5'
48	w	668	A2M	C3'-C4'-C5'-O5'
48	w	799	OMU	C3'-C4'-C5'-O5'
48	w	822	PSU	O4'-C4'-C5'-O5'
48	w	1238	PSU	O4'-C4'-C5'-O5'
48	w	1639	G7M	C3'-C4'-C5'-O5'
48	w	1703	OMC	O4'-C4'-C5'-O5'
3	D	4447	5MC	C2'-C1'-N1-C6
3	D	3701	OMC	C2'-C1'-N1-C2
48	w	34	PSU	O4'-C4'-C5'-O5'
48	w	799	OMU	O4'-C4'-C5'-O5'
3	D	4447	5MC	C2'-C1'-N1-C2
2	B	13	PSU	C3'-C4'-C5'-O5'
3	D	2364	OMG	C3'-C4'-C5'-O5'
48	w	1490	OMG	C3'-C4'-C5'-O5'
2	C	53	5MU	O4'-C4'-C5'-O5'
3	D	1677	PSU	O4'-C4'-C5'-O5'
48	w	99	A2M	O4'-C4'-C5'-O5'
48	w	590	A2M	O4'-C4'-C5'-O5'
48	w	590	A2M	C3'-C4'-C5'-O5'
48	w	644	OMG	O4'-C4'-C5'-O5'
48	w	1288	OMU	O4'-C4'-C5'-O5'
48	w	1490	OMG	O4'-C4'-C5'-O5'
3	D	1677	PSU	C3'-C4'-C5'-O5'
48	w	1490	OMG	C4'-C5'-O5'-P
2	C	47	5MC	O4'-C4'-C5'-O5'
3	D	3760	A2M	C3'-C4'-C5'-O5'
3	D	4447	5MC	O4'-C1'-N1-C6
2	C	34	56B	C7-C9-N10-C10
3	D	3701	OMC	O4'-C1'-N1-C6
48	w	644	OMG	C4'-C5'-O5'-P
2	B	6	2MG	O4'-C4'-C5'-O5'
2	B	13	PSU	O4'-C4'-C5'-O5'
48	w	1248	B8N	C31-C32-C33-C34
3	D	2401	A2M	C3'-C2'-O2'-CM'
3	D	4370	OMG	C3'-C2'-O2'-CM2
3	D	4499	OMG	C3'-C2'-O2'-CM2
48	w	172	OMU	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
2	C	47	5MC	C4'-C5'-O5'-P
3	D	3944	OMG	C4'-C5'-O5'-P
3	D	4500	PSU	C4'-C5'-O5'-P
48	w	34	PSU	C4'-C5'-O5'-P
2	C	9	1MA	C3'-C4'-C5'-O5'
48	w	1703	OMC	C3'-C4'-C5'-O5'
3	D	4447	5MC	O4'-C1'-N1-C2
3	D	3701	OMC	O4'-C1'-N1-C2
3	D	3760	A2M	O4'-C4'-C5'-O5'
3	D	3770	PSU	C3'-C4'-C5'-O5'
48	w	428	OMU	O4'-C1'-N1-C6
3	D	1534	A2M	C4'-C5'-O5'-P
48	w	1248	B8N	C32-C33-C34-O35
48	w	1288	OMU	C4'-C5'-O5'-P
48	w	1326	OMU	O4'-C1'-N1-C6
48	w	1248	B8N	C32-C33-C34-O36
2	B	47	5MC	C4'-C5'-O5'-P
48	w	428	OMU	O4'-C1'-N1-C2
48	w	1326	OMU	C2'-C1'-N1-C6
2	C	54	PSU	O4'-C1'-C5-C4
3	D	1677	PSU	O4'-C1'-C5-C4
3	D	3818	UY1	O4'-C1'-C5-C4
3	D	4521	PSU	O4'-C1'-C5-C4
3	D	1625	OMG	C3'-C2'-O2'-CM2
3	D	4494	OMG	C3'-C2'-O2'-CM2
48	w	627	OMU	C2'-C1'-N1-C6
48	w	509	OMG	O4'-C4'-C5'-O5'
2	B	9	1MA	C3'-C4'-C5'-O5'
2	C	9	1MA	O4'-C4'-C5'-O5'
2	C	53	5MU	C3'-C4'-C5'-O5'
48	w	627	OMU	O4'-C1'-N1-C6
2	B	9	1MA	O4'-C4'-C5'-O5'
3	D	398	A2M	O4'-C4'-C5'-O5'
48	w	27	A2M	C1'-C2'-O2'-CM'
48	w	462	OMC	C1'-C2'-O2'-CM2
48	w	1326	OMU	O4'-C1'-N1-C2
3	D	2422	OMC	O4'-C4'-C5'-O5'
48	w	99	A2M	C3'-C4'-C5'-O5'
2	C	54	PSU	O4'-C1'-C5-C6
3	D	1677	PSU	O4'-C1'-C5-C6
3	D	3818	UY1	O4'-C1'-C5-C6
3	D	4521	PSU	O4'-C1'-C5-C6

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Mol	Chain	Res	Type	Atoms
48	w	1326	OMU	C2'-C1'-N1-C2
3	D	3887	OMC	C4'-C5'-O5'-P
3	D	2351	OMC	O4'-C4'-C5'-O5'
48	w	1804	OMU	C3'-C4'-C5'-O5'
3	D	3944	OMG	C3'-C2'-O2'-CM2
2	B	6	2MG	C3'-C4'-C5'-O5'
2	B	34	56B	O4'-C4'-C5'-O5'
3	D	2815	A2M	C4'-C5'-O5'-P
3	D	1524	A2M	C3'-C4'-C5'-O5'
3	D	3851	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 545 ligands modelled in this entry, 545 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

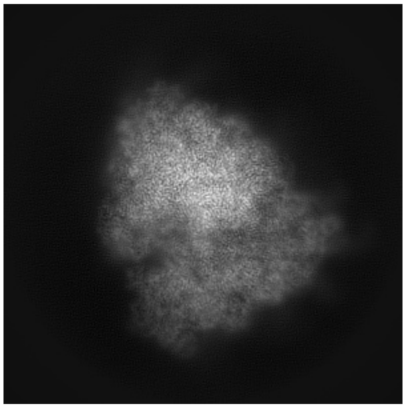
6 Map visualisation ⓘ

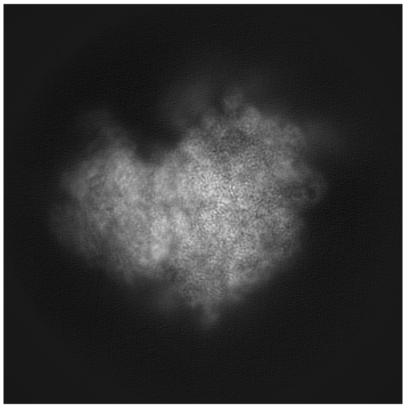
This section contains visualisations of the EMDB entry EMD-36178. These allow visual inspection of the internal detail of the map and identification of artifacts.

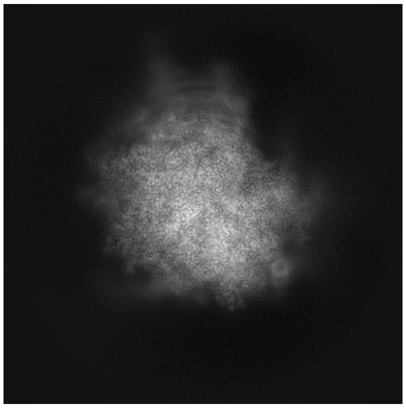
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

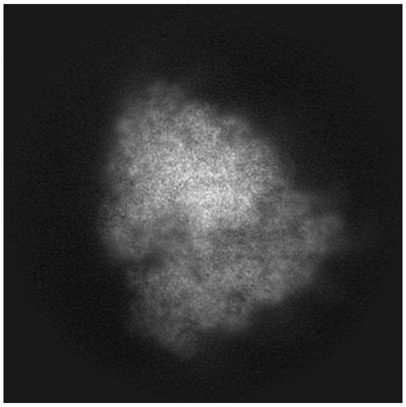
6.1.1 Primary map

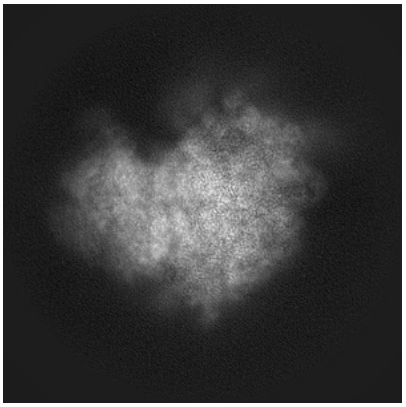

X

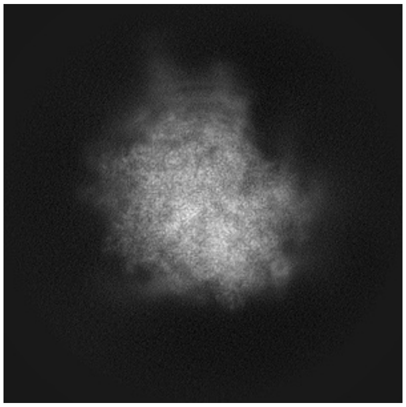

Y


Z

6.1.2 Raw map


X

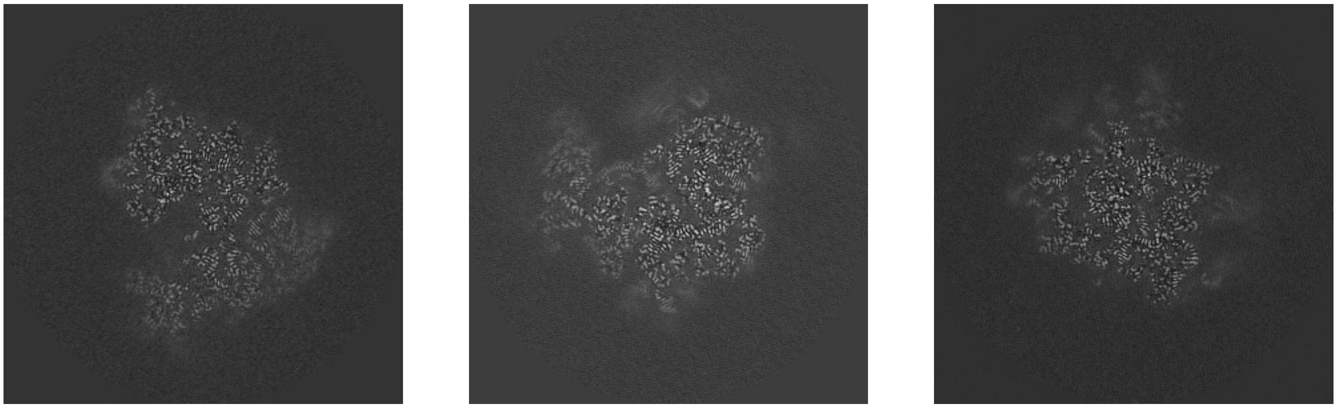

Y


Z

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

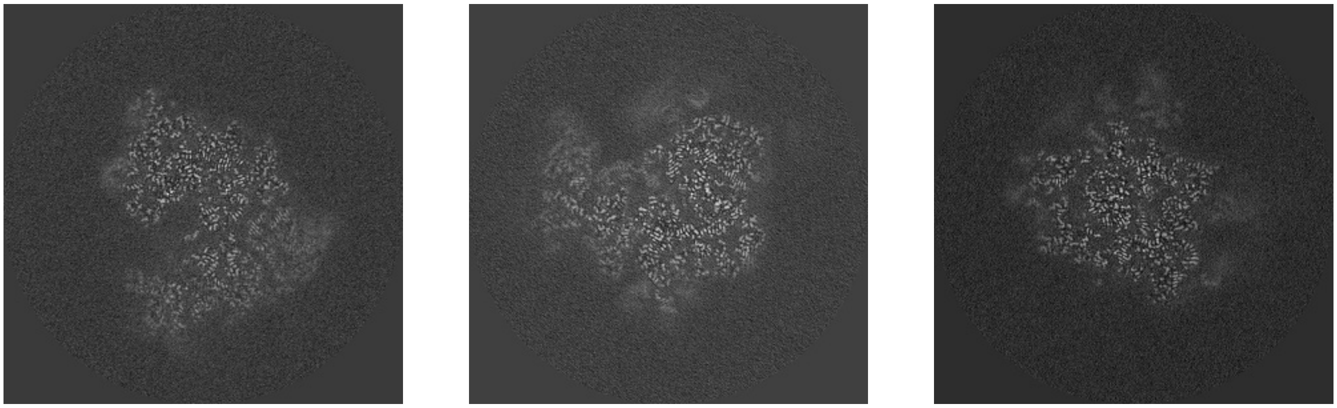
6.2 Central slices (i)

6.2.1 Primary map



X Index: 265 Y Index: 265 Z Index: 265

6.2.2 Raw map

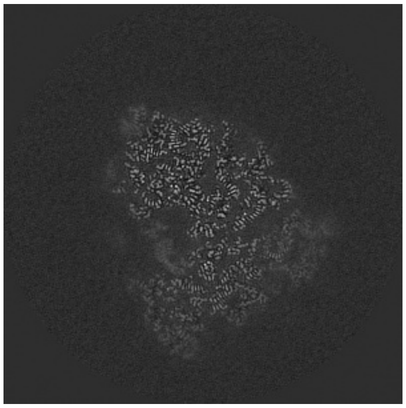


X Index: 265 Y Index: 265 Z Index: 265

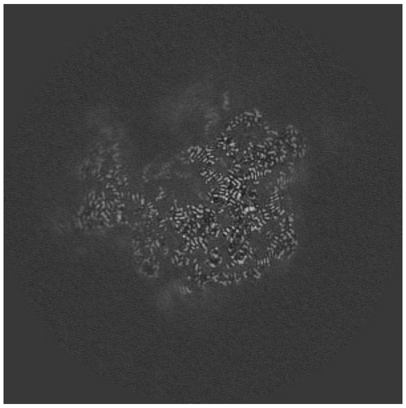
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

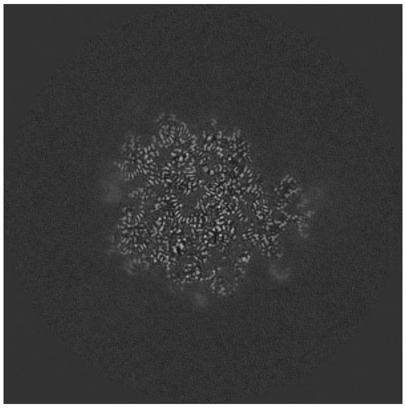
6.3.1 Primary map



X Index: 253

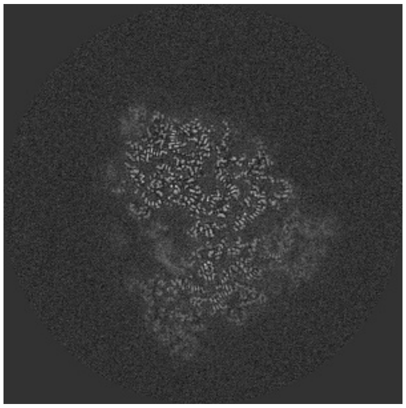


Y Index: 258

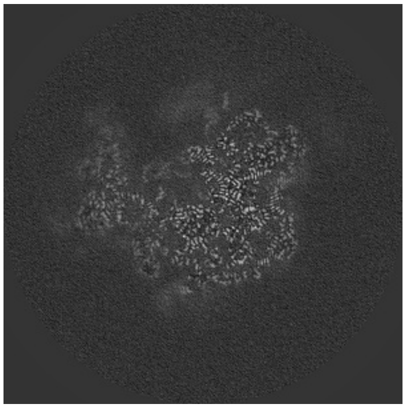


Z Index: 300

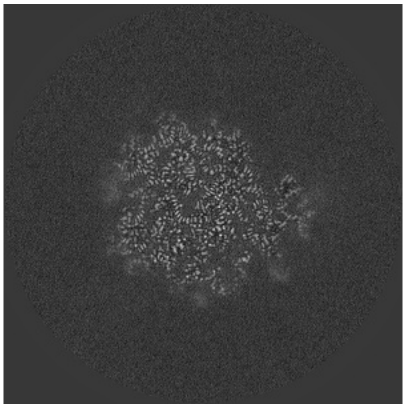
6.3.2 Raw map



X Index: 253



Y Index: 258

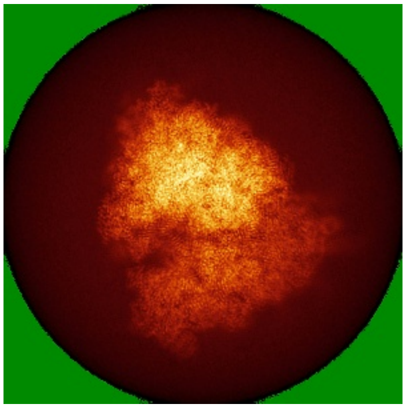


Z Index: 300

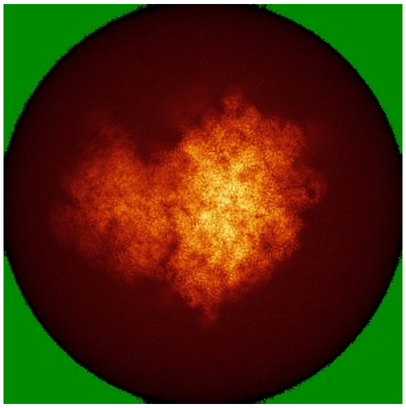
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

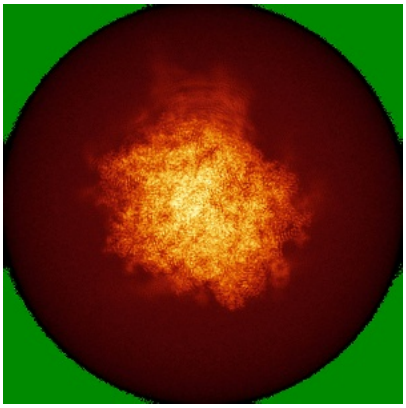
6.4.1 Primary map



X

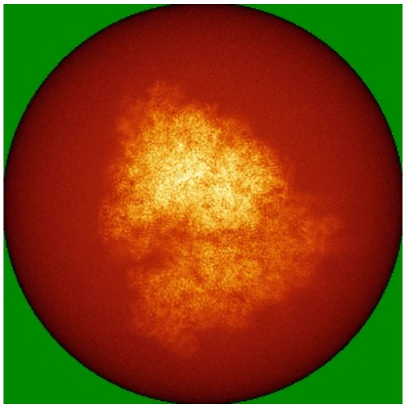


Y

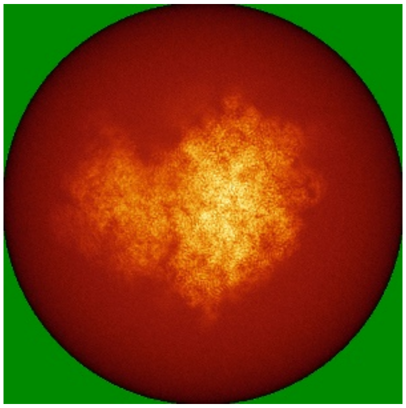


Z

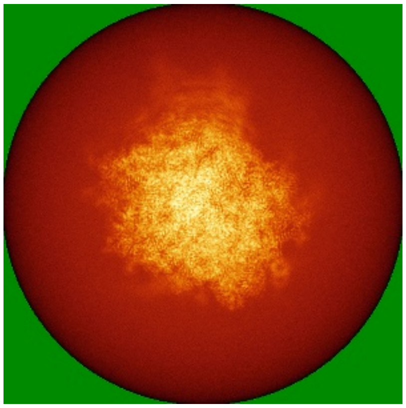
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0204. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

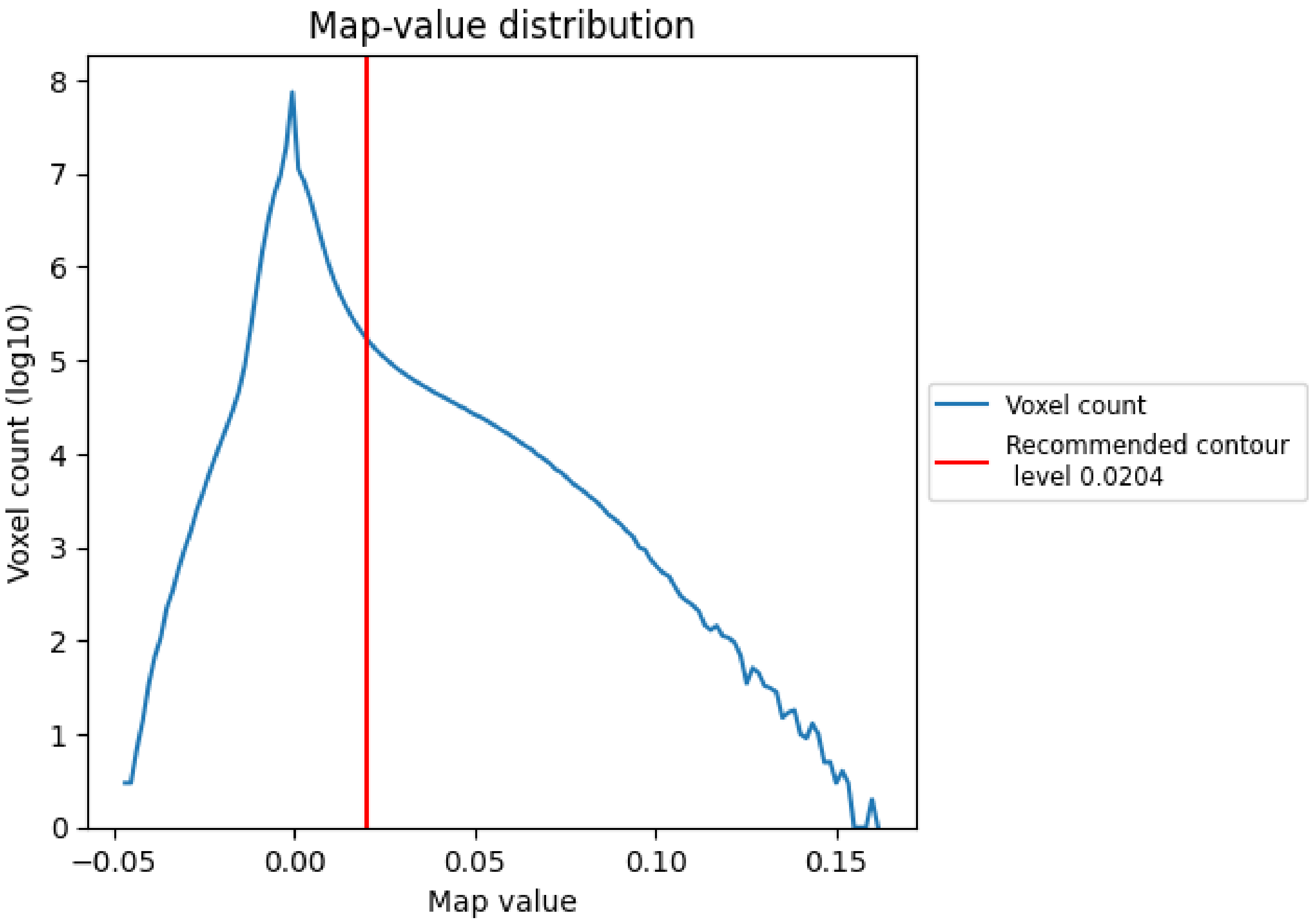
6.6 Mask visualisation

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

7 Map analysis (i)

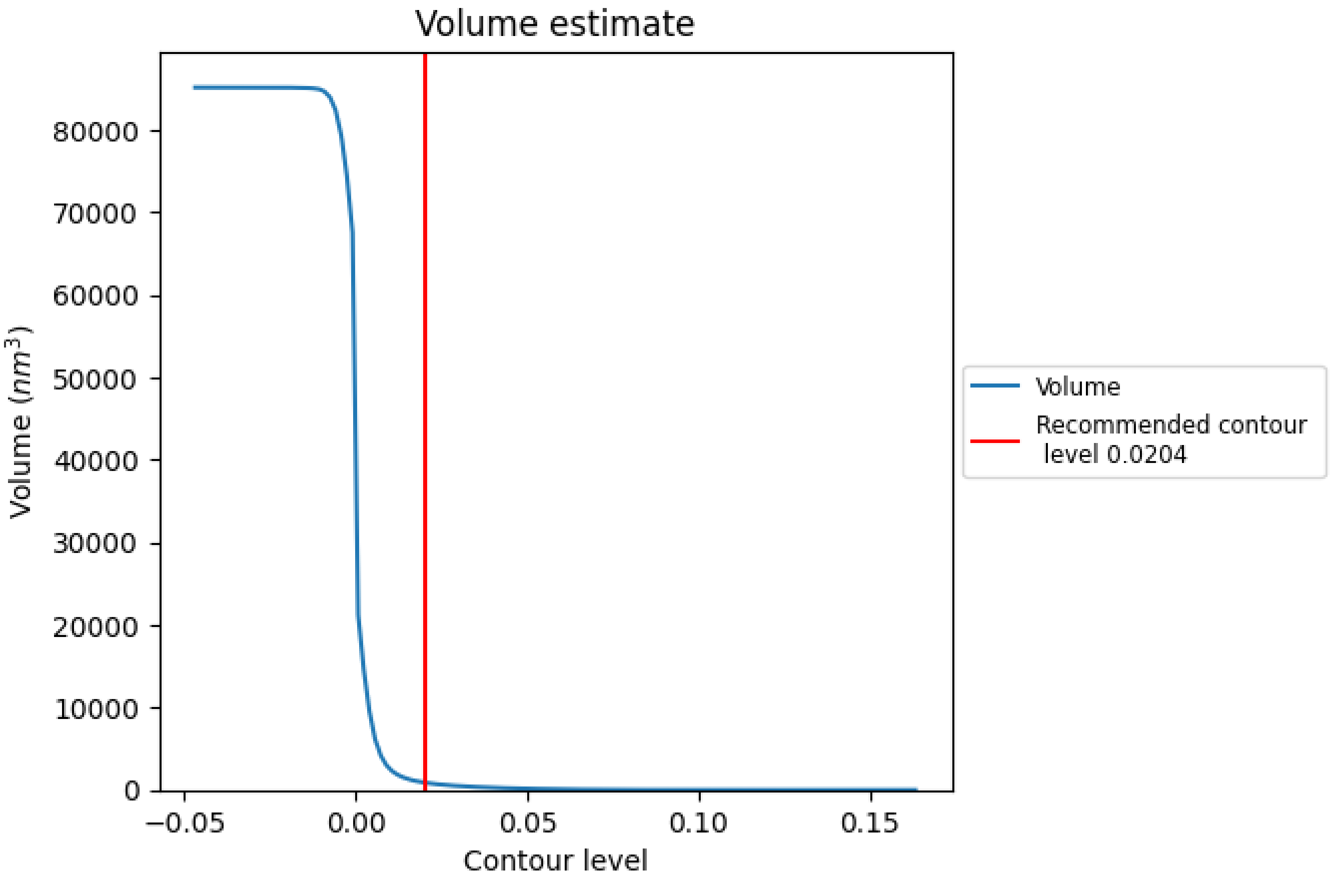
This section contains the results of statistical analysis of the map.

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.

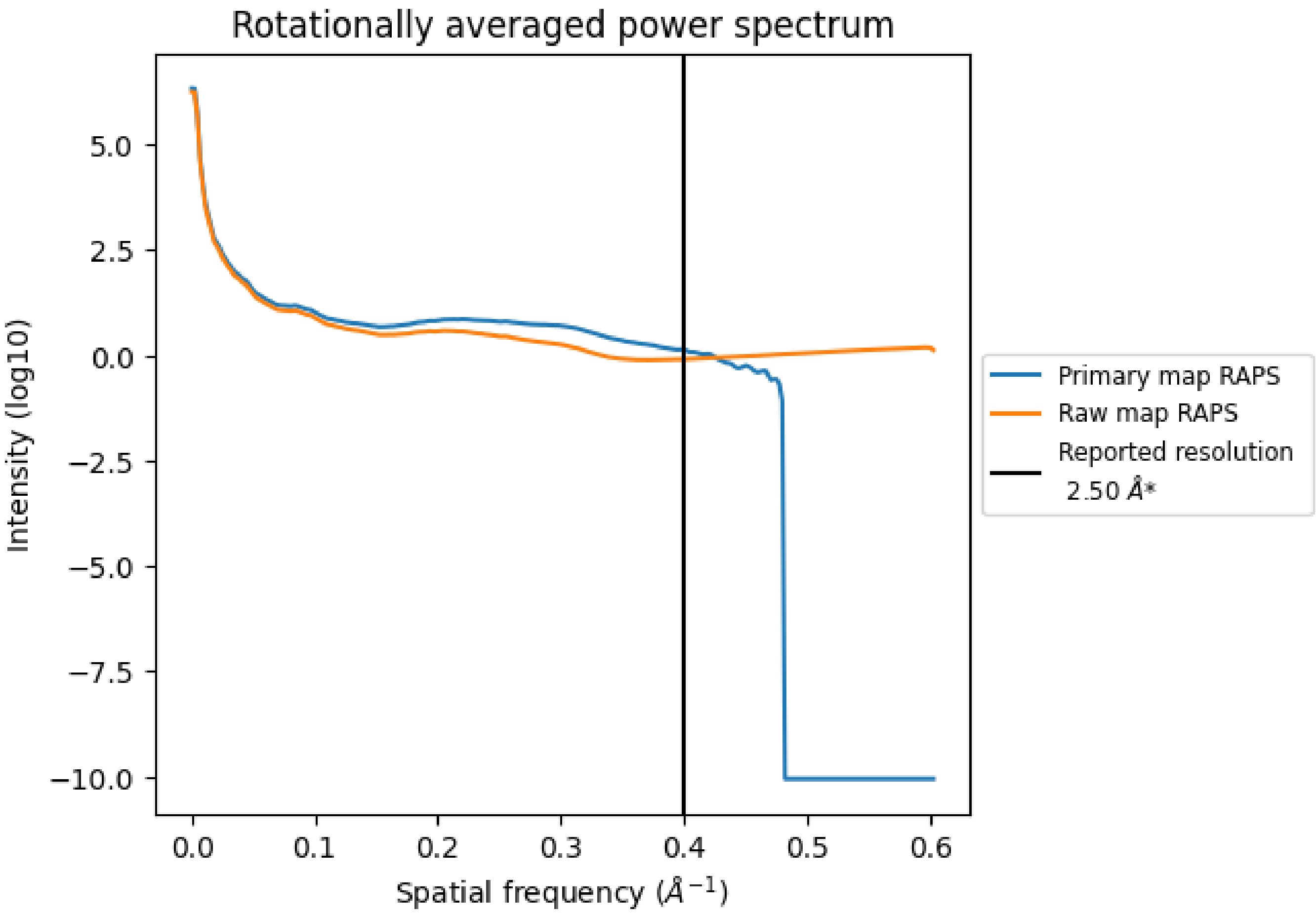
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 872 nm^3; this corresponds to an approximate mass of 788 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

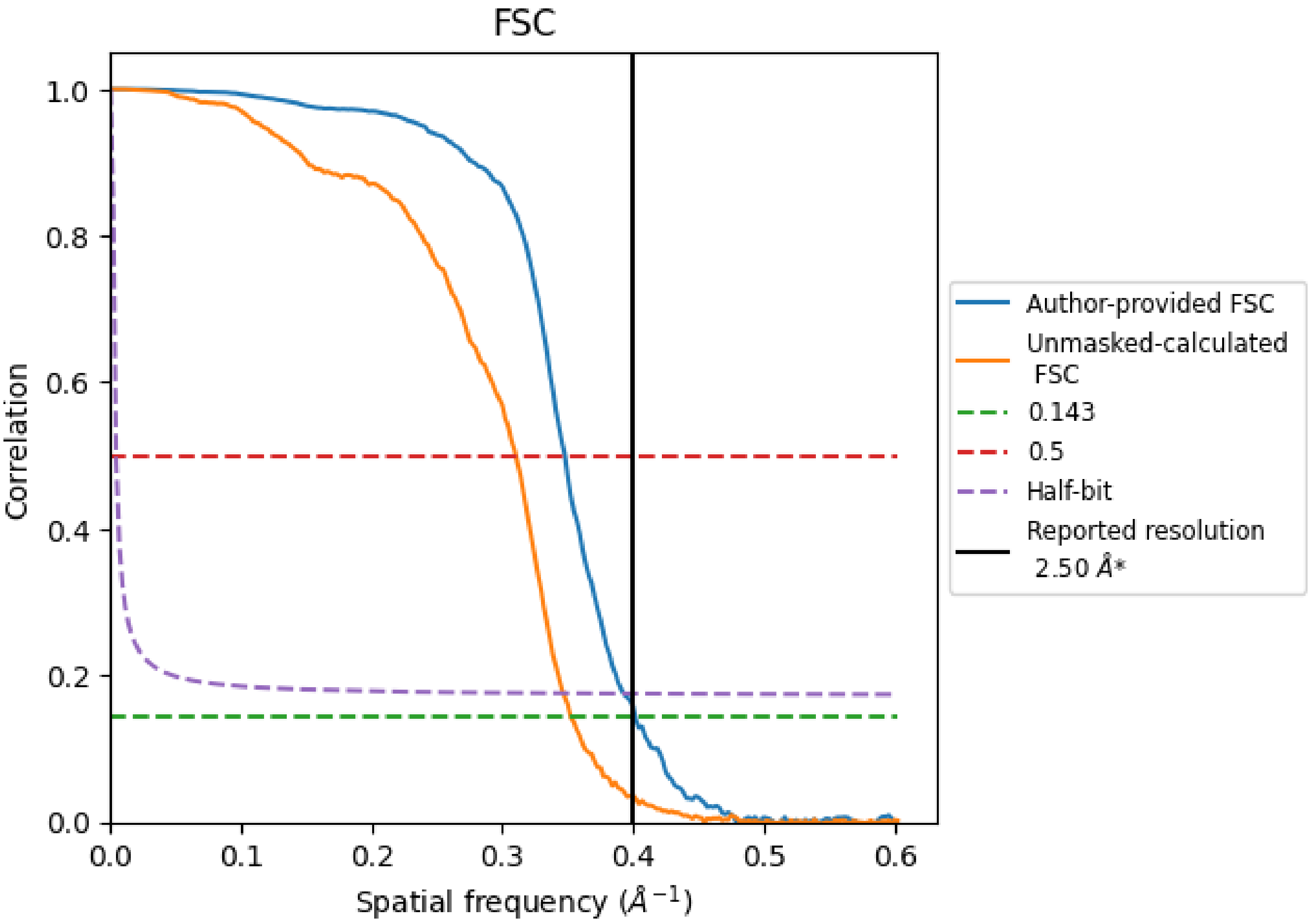


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates ⓘ

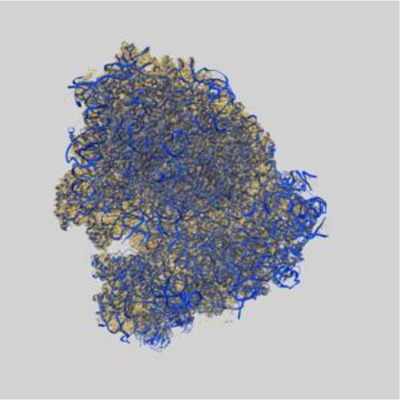
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.87	2.55
Unmasked-calculated*	2.84	3.22	2.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.84 differs from the reported value 2.5 by more than 10 %

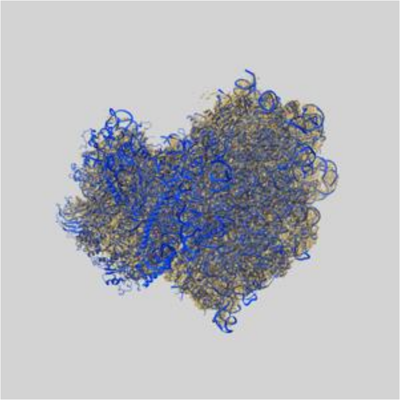
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36178 and PDB model 8JDJ. Per-residue inclusion information can be found in section 3 on page 19.

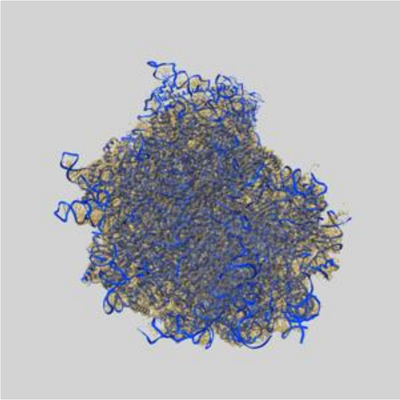
9.1 Map-model overlay



X



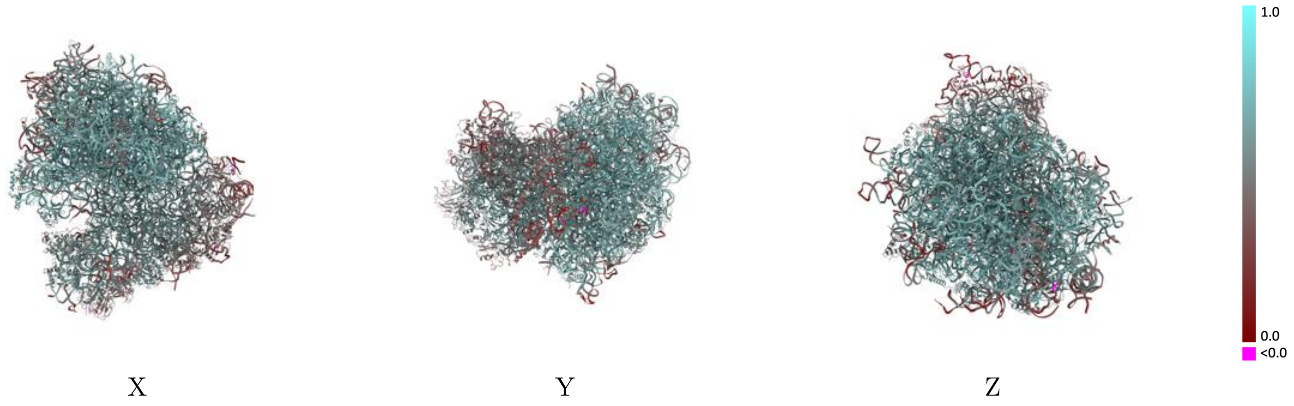
Y



Z

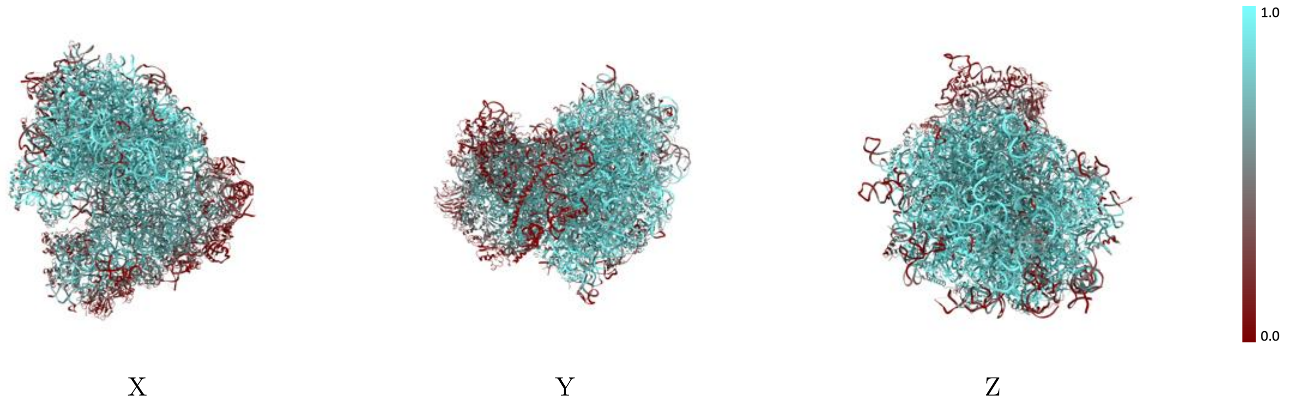
The images above show the 3D surface view of the map at the recommended contour level 0.0204 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



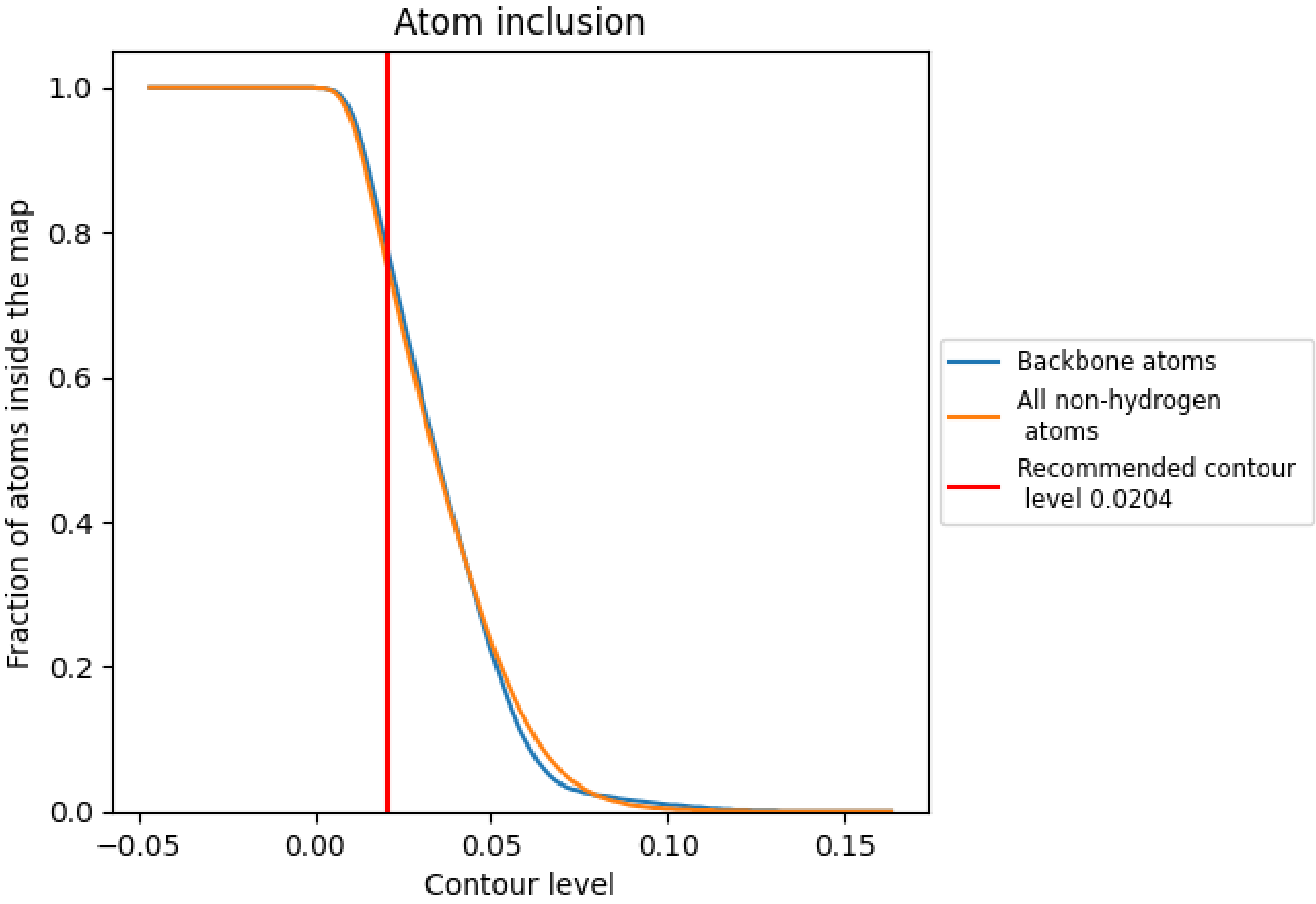
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0204).

9.4 Atom inclusion ⓘ



At the recommended contour level, 78% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7560	0.5940
0	0.4300	0.5030
1	0.1920	0.4160
2	0.5890	0.5570
3	0.1380	0.3760
4	0.2120	0.4330
5	0.4180	0.4690
6	0.2690	0.4200
7	0.1920	0.4090
8	0.5540	0.5380
9	0.6460	0.5830
A	0.7530	0.5730
AA	0.7120	0.5910
AB	0.3450	0.5030
AC	0.5690	0.5560
AD	0.3730	0.4790
AE	0.4660	0.5170
AF	0.5290	0.5460
AG	0.3960	0.4720
AH	0.5030	0.5610
AI	0.7210	0.6100
AJ	0.6570	0.5690
AK	0.0850	0.3780
AL	0.2980	0.4910
AM	0.7380	0.6020
AN	0.4170	0.5080
AO	0.4970	0.5270
AP	0.7720	0.6050
AQ	0.2430	0.4390
AR	0.1450	0.4090
B	0.7340	0.5560
C	0.5610	0.5650
D	0.8550	0.6220
E	0.9800	0.6730
F	0.9010	0.6360

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Chain	Atom inclusion	Q-score
G	0.9550	0.6850
H	0.8850	0.6650
I	0.8960	0.6530
J	0.7930	0.6250
K	0.7470	0.6060
L	0.8990	0.6680
M	0.7090	0.5960
N	0.8330	0.6410
O	0.8630	0.6450
P	0.7060	0.5940
Q	0.8040	0.6270
R	0.8490	0.6380
S	0.9710	0.6860
T	0.9130	0.6740
U	0.8890	0.6690
V	0.9320	0.6750
W	0.7920	0.6230
X	0.9190	0.6720
Y	0.8500	0.6450
Z	0.5790	0.5520
a	0.8970	0.6740
b	0.8780	0.6650
c	0.8270	0.6340
d	0.8200	0.6300
e	0.8170	0.6290
f	0.9170	0.6710
g	0.7080	0.5860
h	0.8250	0.6290
i	0.8220	0.6470
j	0.9330	0.6880
k	0.9370	0.6720
l	0.8510	0.6420
m	0.8160	0.6370
n	0.7680	0.6360
o	0.9550	0.6800
p	0.6550	0.5890
q	0.8960	0.6520
r	0.8750	0.6570
s	0.9130	0.6680
t	0.8330	0.6340
u	0.8800	0.6660
v	0.8920	0.6410

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Chain	Atom inclusion	Q-score
w	▬ 0.7260	▬ 0.5470
x	▬ 0.5390	▬ 0.5670
y	▬ 0.6030	▬ 0.5830
z	▬ 0.6630	▬ 0.5930