



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:47 am GMT

PDB ID : 6HRM
EMDB ID : EMD-0261
Title : E. coli 70S d2d8 stapled ribosome
Authors : Schmied, W.H.; Tnimov, Z.; Uttamapinant, C.; Rae, C.D.; Fried, S.D.; Chin, J.W.
Deposited on : 2018-09-27
Resolution : 2.96 Å(reported)
Based on initial model : 5MDZ

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

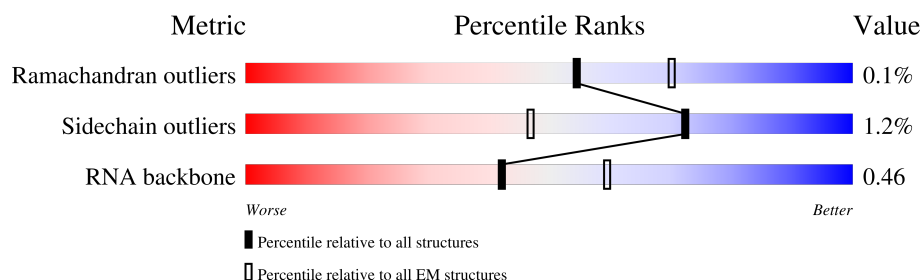
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	4458	<div> <div>15%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
2	3	120	<div> <div>8%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
3	B	271	<div> <div>.</div> <div>98%</div> <div>.</div> </div>
4	C	209	<div> <div>6%</div> <div>99%</div> <div>.</div> </div>
5	D	201	<div> <div>20%</div> <div>99%</div> <div>.</div> </div>
6	E	177	<div> <div>73%</div> <div>98%</div> <div>.</div> </div>
7	F	175	<div> <div>41%</div> <div>98%</div> <div>.</div> </div>
8	G	149	<div> <div>87%</div> <div>98%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	H	130	100%
10	I	135	100%
11	J	142	6%
12	K	123	98%
13	L	144	98%
14	M	136	100%
15	N	119	100%
16	O	116	17%
17	P	114	8%
18	Q	117	99%
19	R	103	10%
20	S	110	6%
21	T	94	15%
22	U	103	29%
23	V	94	20%
24	W	76	99%
25	X	77	8%
26	Y	62	37%
27	Z	58	7%
28	a	66	97%
29	b	56	9%
30	c	52	10%
31	d	46	98%
32	e	64	95%
33	f	38	8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	g	225	80% 100%
35	h	208	61% 99%
36	i	205	46% 100%
37	j	156	22% 97%
38	k	104	35% 98%
39	l	151	87% 99%
40	m	129	20% 98%
41	n	127	83% 98%
42	o	99	82% 99%
43	p	117	34% 98%
44	q	123	15% 98%
45	r	116	89% 100%
46	s	100	64% 100%
47	t	88	22% 95% 5%
48	u	82	26% 99%
49	v	80	32% 98%
50	w	66	17% 100%
51	x	83	94% 98%
52	y	86	21% 99%
53	z	70	83% 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	4OC	1	1402	X	-	-	-
1	1MG	1	2251	X	-	-	-
1	PSU	1	2252	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	5MU	1	2253	X	-	-	-
1	PSU	1	2461	X	-	-	-
1	6MZ	1	3124	X	-	-	-
1	PSU	1	3417	X	-	-	-
1	3TD	1	3421	X	-	-	-
1	PSU	1	3423	X	-	-	-
1	5MU	1	3445	X	-	-	-
1	6MZ	1	3536	X	-	-	-
1	G7M	1	3575	X	-	-	-
1	OMG	1	3757	X	-	-	-
1	PSU	1	3963	X	-	-	-
1	OMC	1	4004	X	-	-	-
1	2MA	1	4009	X	-	-	-
1	PSU	1	4010	X	-	-	-
1	OMU	1	4058	X	-	-	-
1	PSU	1	4086	X	-	-	-
1	PSU	1	4111	X	-	-	-
1	PSU	1	516	X	-	-	-
1	7MG	1	527	X	-	-	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 145179 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 stapled 16S-23S rRNA,stapled 16S-23S rRNA,stapled 16S-23S rRNA,stapled 16S-23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	4450	Total	C	N	O	P	0	0
			95544	42634	17562	30898	4450		

There are 153 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1450	G	-	linker	GB 1370526422
1	1451	G	-	linker	GB 1370526422
1	1452	U	-	linker	GB 1370526422
1	1453	C	-	linker	GB 1370526422
1	1454	A	-	linker	GB 1370526422
1	1455	A	-	linker	GB 1370526422
1	1456	C	-	linker	GB 1370526422
1	1457	A	-	linker	GB 1370526422
1	1458	G	-	linker	GB 1370526422
1	1459	C	-	linker	GB 1370526422
1	1460	C	-	linker	GB 1370526422
1	1461	G	-	linker	GB 1370526422
1	1462	U	-	linker	GB 1370526422
1	1463	U	-	linker	GB 1370526422
1	1464	U	-	linker	GB 1370526422
1	1465	G	-	linker	GB 1370526422
1	1466	A	-	linker	GB 1370526422
1	1467	G	-	linker	GB 1370526422
1	1468	C	-	linker	GB 1370526422
1	1469	U	-	linker	GB 1370526422
1	1470	A	-	linker	GB 1370526422
1	1471	A	-	linker	GB 1370526422
1	1472	C	-	linker	GB 1370526422
1	1473	C	-	linker	GB 1370526422
1	1474	G	-	linker	GB 1370526422
1	1475	G	-	linker	GB 1370526422
1	1476	U	-	linker	GB 1370526422

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1	1477	A	-	linker	GB 1370526422
1	1478	C	-	linker	GB 1370526422
1	1479	U	-	linker	GB 1370526422
1	1480	A	-	linker	GB 1370526422
1	1481	A	-	linker	GB 1370526422
1	1482	U	-	linker	GB 1370526422
1	1483	G	-	linker	GB 1370526422
1	1484	A	-	linker	GB 1370526422
1	1485	A	-	linker	GB 1370526422
1	1486	C	-	linker	GB 1370526422
1	1487	C	-	linker	GB 1370526422
1	1488	G	-	linker	GB 1370526422
1	1489	U	-	linker	GB 1370526422
1	1490	G	-	linker	GB 1370526422
1	1491	A	-	linker	GB 1370526422
1	1492	G	-	linker	GB 1370526422
1	1493	G	-	linker	GB 1370526422
1	1494	C	-	linker	GB 1370526422
1	1495	U	-	linker	GB 1370526422
1	1496	U	-	linker	GB 1370526422
1	1497	A	-	linker	GB 1370526422
1	1498	A	-	linker	GB 1370526422
1	1499	C	-	linker	GB 1370526422
1	1500	C	-	linker	GB 1370526422
1	1504	A	U	conflict	GB 1063812051
1	4358	A	-	expression tag	GB 1063812051
1	4359	C	-	expression tag	GB 1063812051
1	4360	G	-	expression tag	GB 1063812051
1	4361	G	-	expression tag	GB 1063812051
1	4362	A	-	expression tag	GB 1063812051
1	4363	C	-	expression tag	GB 1063812051
1	4364	A	-	expression tag	GB 1063812051
1	4365	U	-	expression tag	GB 1063812051
1	4366	G	-	expression tag	GB 1063812051
1	4367	G	-	expression tag	GB 1063812051
1	4368	U	-	expression tag	GB 1063812051
1	4369	U	-	expression tag	GB 1063812051
1	4370	G	-	expression tag	GB 1063812051
1	4371	G	-	expression tag	GB 1063812051
1	4372	A	-	expression tag	GB 1063812051
1	4373	G	-	expression tag	GB 1063812051
1	4374	G	-	expression tag	GB 1063812051

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1	4375	G	-	expression tag	GB 1063812051
1	4376	C	-	expression tag	GB 1063812051
1	4377	G	-	expression tag	GB 1063812051
1	4378	C	-	expression tag	GB 1063812051
1	4379	U	-	expression tag	GB 1063812051
1	4380	U	-	expression tag	GB 1063812051
1	4381	A	-	expression tag	GB 1063812051
1	4382	C	-	expression tag	GB 1063812051
1	4383	C	-	expression tag	GB 1063812051
1	4384	A	-	expression tag	GB 1063812051
1	4385	C	-	expression tag	GB 1063812051
1	4386	U	-	expression tag	GB 1063812051
1	4387	U	-	expression tag	GB 1063812051
1	4388	U	-	expression tag	GB 1063812051
1	4389	G	-	expression tag	GB 1063812051
1	4390	U	-	expression tag	GB 1063812051
1	4391	G	-	expression tag	GB 1063812051
1	4392	A	-	expression tag	GB 1063812051
1	4393	U	-	expression tag	GB 1063812051
1	4394	U	-	expression tag	GB 1063812051
1	4395	C	-	expression tag	GB 1063812051
1	4396	A	-	expression tag	GB 1063812051
1	4397	U	-	expression tag	GB 1063812051
1	4398	G	-	expression tag	GB 1063812051
1	4399	A	-	expression tag	GB 1063812051
1	4400	C	-	expression tag	GB 1063812051
1	4401	U	-	expression tag	GB 1063812051
1	4402	G	-	expression tag	GB 1063812051
1	4403	G	-	expression tag	GB 1063812051
1	4404	G	-	expression tag	GB 1063812051
1	4405	G	-	expression tag	GB 1063812051
1	4406	U	-	expression tag	GB 1063812051
1	4407	G	-	expression tag	GB 1063812051
1	4408	A	-	expression tag	GB 1063812051
1	4409	A	-	expression tag	GB 1063812051
1	4410	G	-	expression tag	GB 1063812051
1	4411	U	-	expression tag	GB 1063812051
1	4412	C	-	expression tag	GB 1063812051
1	4413	G	-	expression tag	GB 1063812051
1	4414	UR3	-	expression tag	GB 1063812051
1	4415	A	-	expression tag	GB 1063812051
1	4416	A	-	expression tag	GB 1063812051

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
1	4417	C	-	expression tag	GB 1063812051
1	4418	A	-	expression tag	GB 1063812051
1	4419	A	-	expression tag	GB 1063812051
1	4420	G	-	expression tag	GB 1063812051
1	4421	G	-	expression tag	GB 1063812051
1	4422	U	-	expression tag	GB 1063812051
1	4423	A	-	expression tag	GB 1063812051
1	4424	A	-	expression tag	GB 1063812051
1	4425	C	-	expression tag	GB 1063812051
1	4426	C	-	expression tag	GB 1063812051
1	4427	G	-	expression tag	GB 1063812051
1	4428	U	-	expression tag	GB 1063812051
1	4429	A	-	expression tag	GB 1063812051
1	4430	G	-	expression tag	GB 1063812051
1	4431	G	-	expression tag	GB 1063812051
1	4432	2MG	-	expression tag	GB 1063812051
1	4433	G	-	expression tag	GB 1063812051
1	4434	MA6	-	expression tag	GB 1063812051
1	4435	MA6	-	expression tag	GB 1063812051
1	4436	C	-	expression tag	GB 1063812051
1	4437	C	-	expression tag	GB 1063812051
1	4438	U	-	expression tag	GB 1063812051
1	4439	G	-	expression tag	GB 1063812051
1	4440	C	-	expression tag	GB 1063812051
1	4441	G	-	expression tag	GB 1063812051
1	4442	G	-	expression tag	GB 1063812051
1	4443	U	-	expression tag	GB 1063812051
1	4444	U	-	expression tag	GB 1063812051
1	4445	G	-	expression tag	GB 1063812051
1	4446	G	-	expression tag	GB 1063812051
1	4447	A	-	expression tag	GB 1063812051
1	4448	U	-	expression tag	GB 1063812051
1	4449	C	-	expression tag	GB 1063812051
1	4450	A	-	expression tag	GB 1063812051
1	4451	C	-	expression tag	GB 1063812051
1	4452	C	-	expression tag	GB 1063812051
1	4453	U	-	expression tag	GB 1063812051
1	4454	C	-	expression tag	GB 1063812051
1	4455	C	-	expression tag	GB 1063812051
1	4456	U	-	expression tag	GB 1063812051
1	4457	U	-	expression tag	GB 1063812051
1	4458	A	-	expression tag	GB 1063812051

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	103	Total	C	N	O	0	0
			788	498	148	142		

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	m	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	n	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	p	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	1	422	Total	Mg	0
			422	422	
54	3	8	Total	Mg	0
			8	8	
54	N	1	Total	Mg	0
			1	1	
54	P	1	Total	Mg	0
			1	1	
54	Q	1	Total	Mg	0
			1	1	
54	U	1	Total	Mg	0
			1	1	
54	b	1	Total	Mg	0
			1	1	
54	i	1	Total	Mg	0
			1	1	

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	a	1	Total	Zn	0
			1	1	
55	f	1	Total	Zn	0
			1	1	

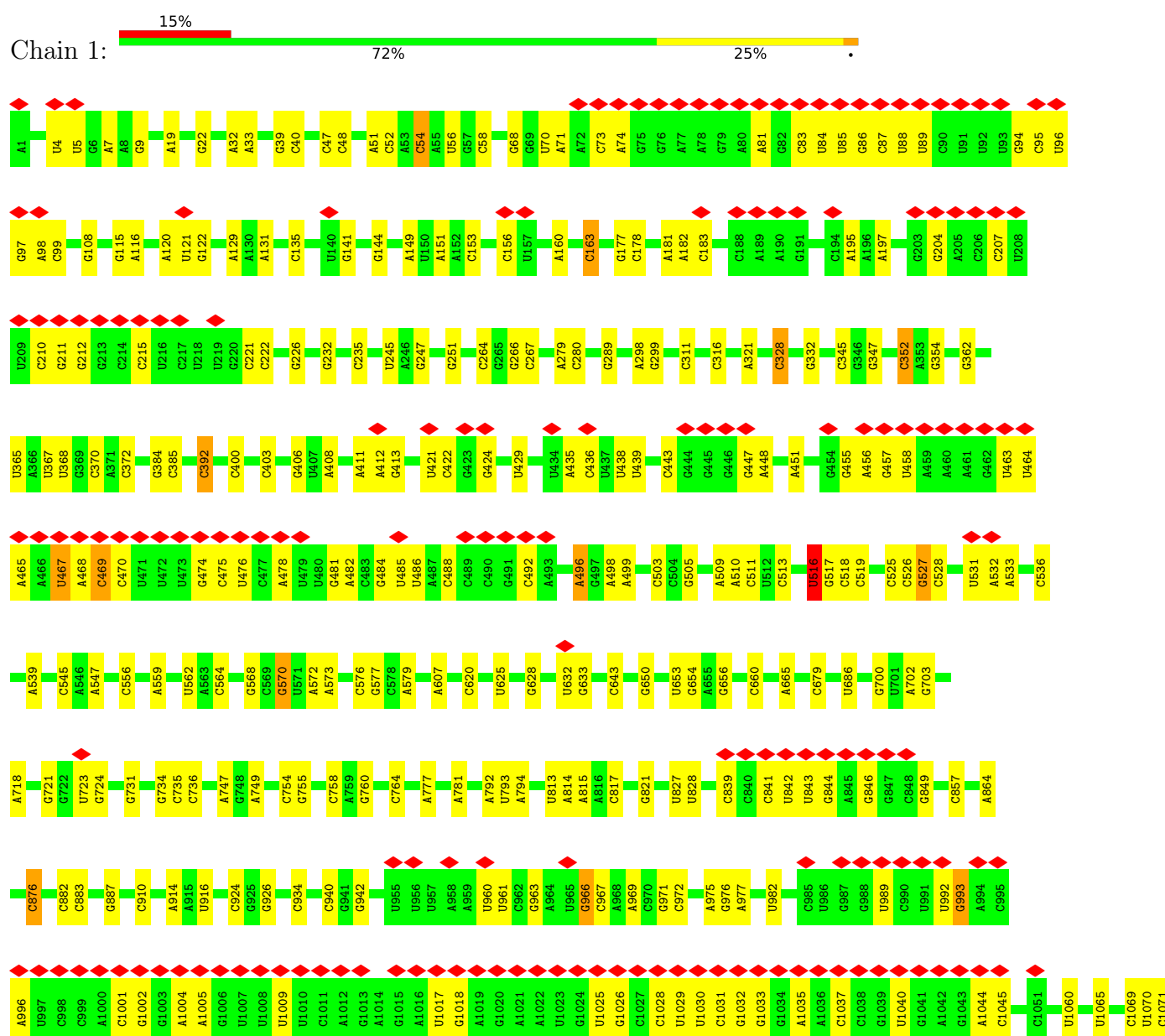
- Molecule 56 is water.

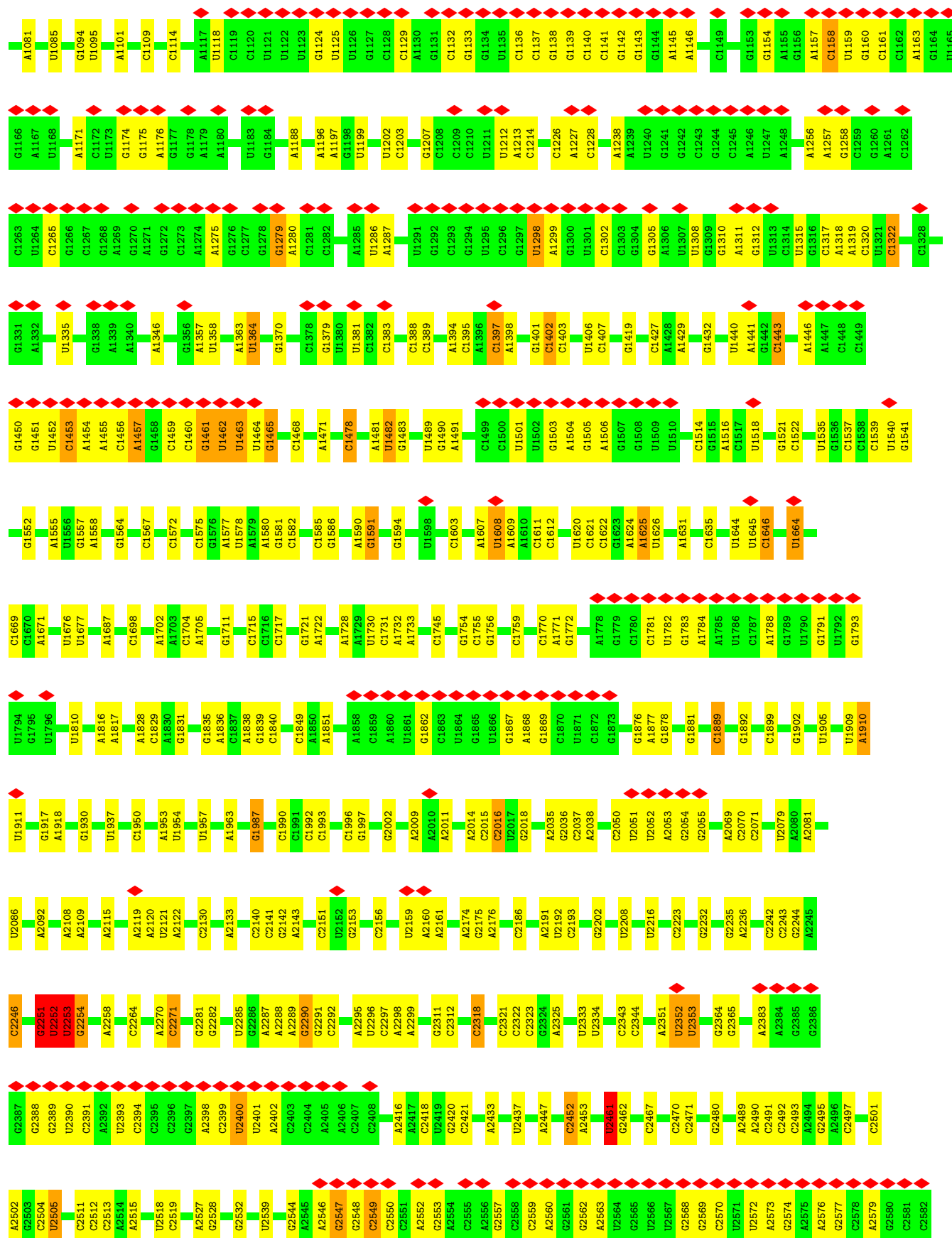
Mol	Chain	Residues	Atoms		AltConf
56	B	2	Total	O	0
			2	2	

3 Residue-property plots

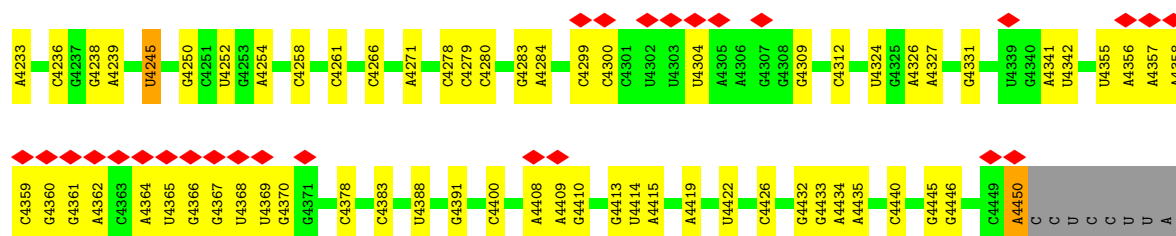
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: stapled 16S-23S rRNA, stapled 16S-23S rRNA, stapled 16S-23S rRNA, stapled 16S-23S rRNA

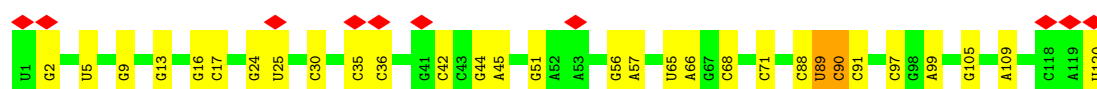
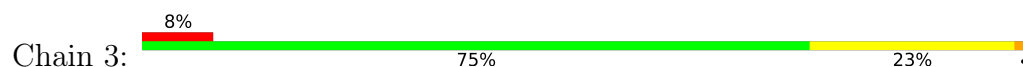




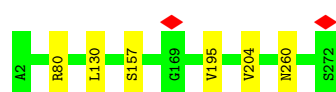
G4075	G3950	C3816	G3692	A3632	G3533	A3422	C3270	U3095	C2967	C2821	C2687	A2583
A4078	G3951	A3817	U3693	G3633	A3536	A3423	C3274	A3096	C2968	A2827	C2676	U2584
C4079	A3954	U3818	U3694	G3634	A3537	A3424	C3274	C3113	C2969	G2830	A2675	C2585
G4080	C3962	G3825	U3695	C3635	C3538	C3425	A3279	C3114	G2984	U2835	C2676	A2586
C4085	U3963	G3826	G3696	U3636	U3540	C3426	C3280	A3115	G2988	C2836	C2677	U2587
U4086	G3964	A3828	A3697	U3637	G3541	U3429	U3281	A3116	U2992	U2846	C2678	U2588
G4087	C3969	G3831	U3698	U3638	G3542	C3430	G3282	A3124	C2995	U2846	U2679	U2589
G4088	C3970	C3832	G3699	G3639	C3550	G3435	U3285	G3125	A2996	U2850	U2680	A2590
C4091	C3971	A3833	U3700	A3640	C3551	G3436	A3280	A3136	C2999	C2851	U2681	A2591
A4095	G3976	U3839	A3704	A3642	G3552	C3440	A3280	A3136	C2999	C2851	U2682	A2592
A4096	G3977	U3840	G3710	G3642	C3553	G3441	C3301	A3140	C2999	C2851	U2682	A2592
C4097	U3979	G3851	U3716	U3643	C3553	G3442	C3301	A3140	C2999	C2851	U2682	A2592
C4100	C3981	A3852	A3717	G3644	C3556	A3443	C3306	C3145	U3003	C2854	G2683	G2593
A4108	U3983	G3857	A3718	G3646	G3562	A3444	A3307	C3145	C3004	C2855	C2684	A2594
U4111	C3984	C3858	U3719	G3647	A3566	U3445	A3308	C3150	A3009	U2858	U2686	A2595
C4112	A3986	A3859	U3726	A3648	A3567	U3446	A3314	U3153	A3010	C2868	U2687	G2597
U4115	G3996	G3860	G3727	G3650	A3568	C3453	G3317	G3155	A3011	C2869	G2692	C2598
U4119	U3997	C3861	C3728	C3651	G3575	U3461	G3322	A3156	U3012	A2871	A2710	U2600
A4003	A4003	G3867	A3731	C3652	C3578	U3462	G3323	G3162	A3013	G2874	G2718	A2601
C4004	C4004	C3868	C3732	A3653	C3579	C3463	G3323	C3162	A3014	G2880	G2718	A2602
C4005	C4005	C3886	U3739	G3654	G3599	C3464	C3328	G3173	A3016	U2881	G2743	U2603
G4008	G4008	C3889	G3744	U3655	G3602	C3468	A3335	A3174	A3021	C2882	G2744	A2604
A4009	A4009	U3889	G3744	C3656	A3603	C3471	C3339	A3175	G3027	U2885	G2745	G2605
U4010	U4010	U3890	U3749	U3657	U3604	C3472	U3340	C3176	A3028	C2886	U2746	G2606
G4011	C3891	G3891	U3749	G3658	U3605	C3473	G3341	G3180	U3029	G2889	G2756	U2607
U4012	U4012	C3896	G3756	C3659	G3606	A3476	C3342	C3181	G3030	U2900	G2756	C2608
C4018	C4018	G3897	G3757	A3660	A3607	U3477	A3353	G3197	C3037	A2901	A2759	A2609
C4021	C4021	G3902	C3766	U3661	G3608	G3478	A3354	C3197	A3038	U2902	G2762	C2610
A4024	A4024	U3908	C3767	G3662	C3609	G3486	U3370	U3220	C3039	U2903	C2763	U2611
U4025	U4025	C3909	C3770	G3663	C3610	A3487	U3371	G3221	C3040	C2904	G2772	G2612
C4026	C4026	U3910	A3774	A3664	U3611	U3488	C3376	G3230	U3041	C2905	U2773	U2614
G4031	G4031	G3911	A3774	G3665	U3612	U3488	C3376	G3230	A3042	U2917	A2774	C2615
G4035	G4035	A3912	A3779	C3666	G3613	C3496	A3406	G3233	C3044	C2920	G2777	A2617
A4053	A4053	U3929	A3784	C3667	A3614	U3497	A3406	C3233	G3044	U2921	A2780	G2618
U4058	U4058	C3930	A3784	G3668	U3615	G3498	C3385	C3234	U3045	C2922	A2781	G2621
G4059	G4059	A3931	C3789	A3669	G3616	U3499	C3385	U3235	G3046	C2923	A2790	C2622
U4060	U4060	C3932	C3789	C3670	U3617	C3500	A3406	C3236	C3047	A2925	A2790	C2623
C4062	C4062	G3935	G3792	C3671	G3618	C3503	A3406	G3237	C3063	A2926	A2791	C2624
U4068	U4068	A3936	A3793	U3672	U3619	G3508	C3411	C3238	C3066	C2934	A2792	U2625
G4072	G4072	C3937	U3803	U3673	A3620	G3512	G3412	G3239	G3072	C2934	A2792	G2626
A4073	A4073	A3677	U3811	G3674	G3621	C3512	G3413	G3240	A3075	C2934	C2795	C2627
C3948	C3948	U3678	G3812	A3675	G3622	C3512	G3413	G3240	U3084	C2934	C2795	G2628
U4074	U4074	G3813	U3808	A3676	A3623	C3527	G3416	U3242	A3089	U2819	C2803	A2632
C4229	C4229	G3814	U3811	A3677	U3624	C3528	A3418	G3243	U3090	C2820	C2804	U2638
A4231	A4231	A3815	G3815	U3678	A3625	C3529	A3419	G3244	C3091	C2641	G2806	A2639
A4232	A4232	A3690	A3691	U3688	G3626	C3529	C3420	A3263	A3092	G2642	A2807	C2640
												A2648
												A2662
												G2663



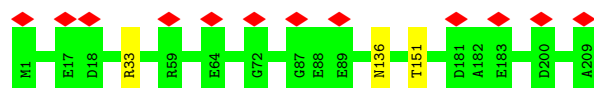
• Molecule 2: 5S ribosomal RNA



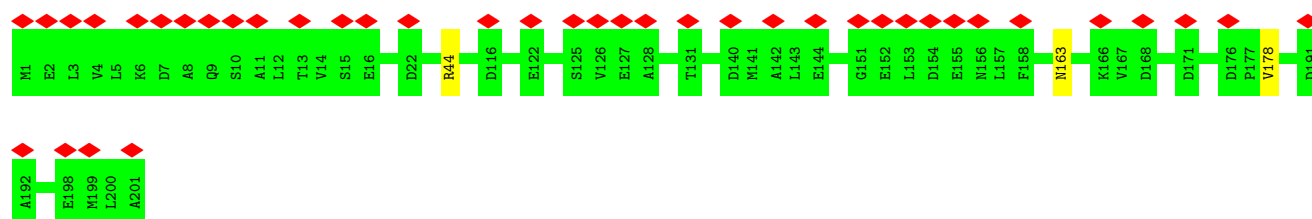
• Molecule 3: 50S ribosomal protein L2



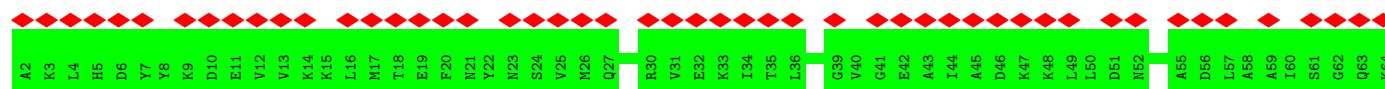
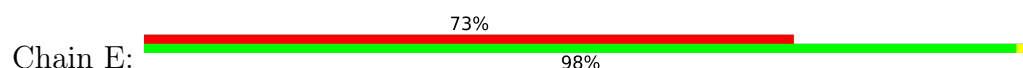
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

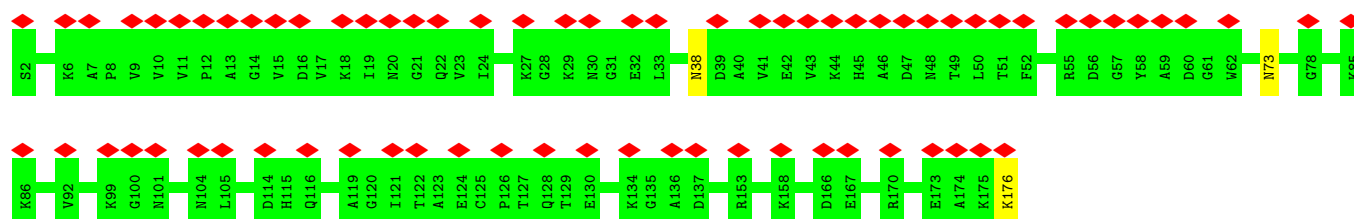
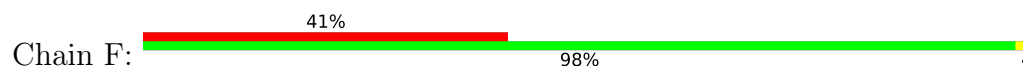


• Molecule 6: 50S ribosomal protein L5

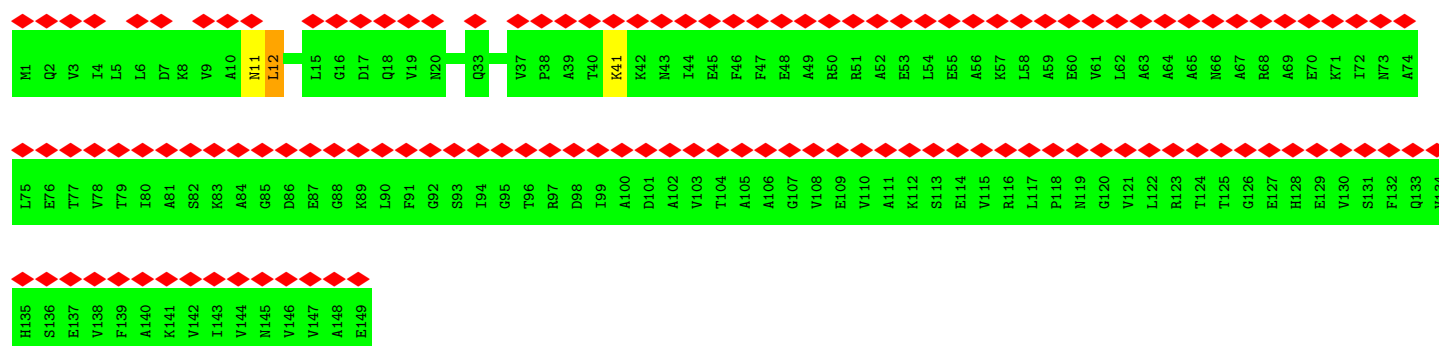
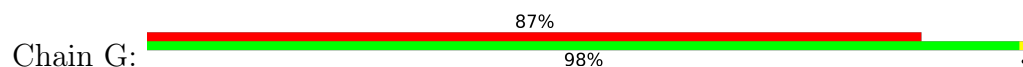




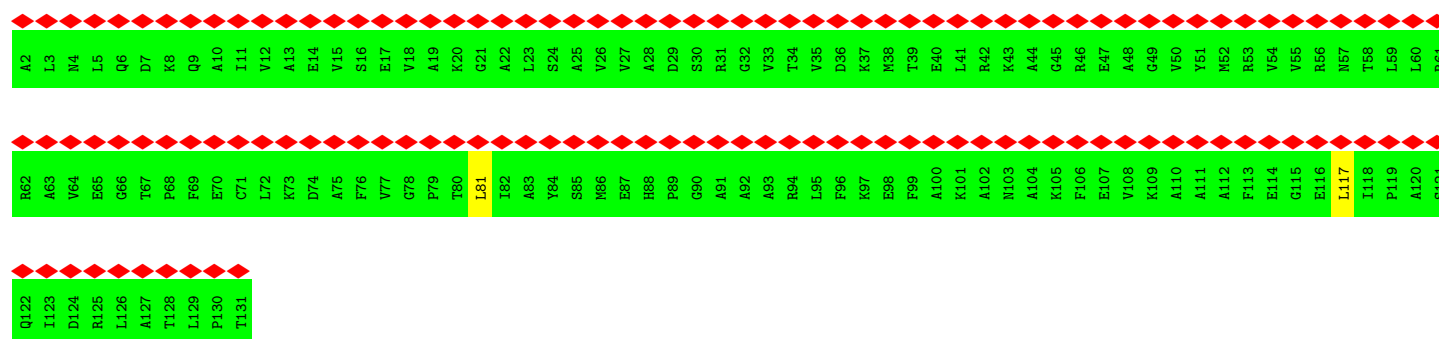
• Molecule 7: 50S ribosomal protein L6



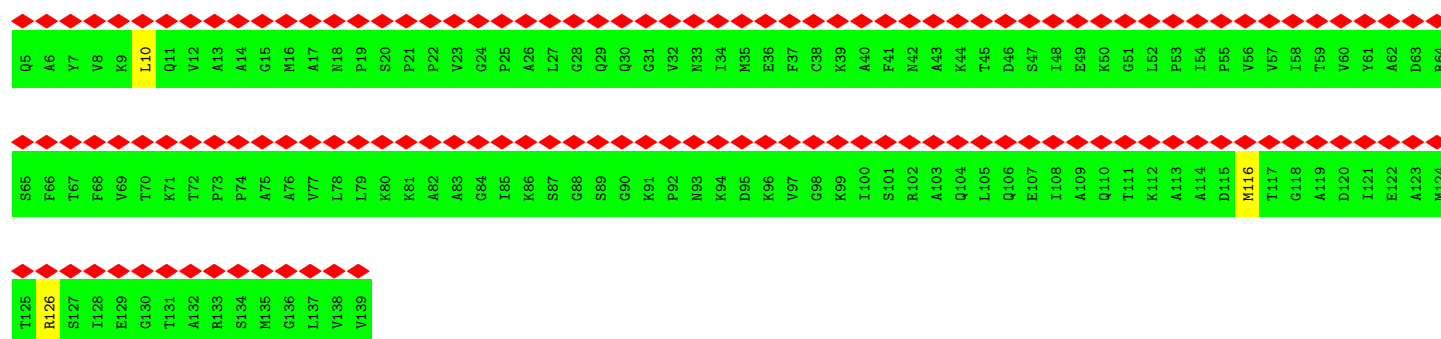
• Molecule 8: 50S ribosomal protein L9



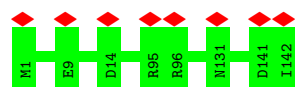
• Molecule 9: 50S ribosomal protein L10



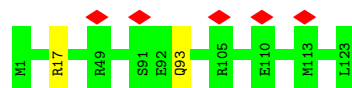
• Molecule 10: 50S ribosomal protein L11



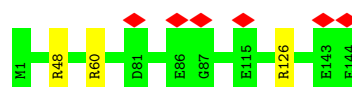
- Molecule 11: 50S ribosomal protein L13



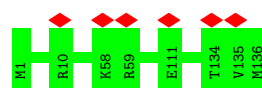
- Molecule 12: 50S ribosomal protein L14



- Molecule 13: 50S ribosomal protein L15



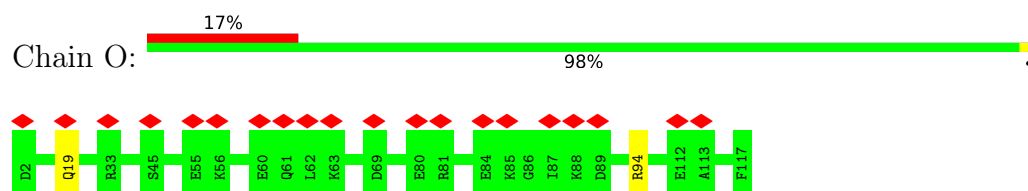
- Molecule 14: 50S ribosomal protein L16



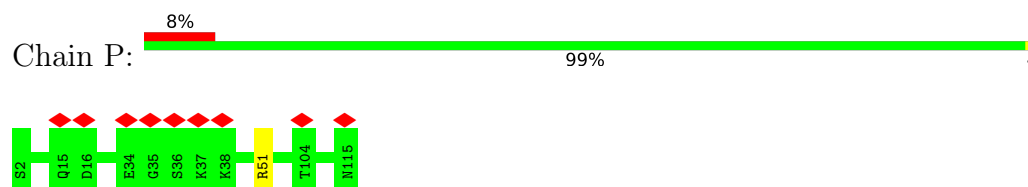
- Molecule 15: 50S ribosomal protein L17



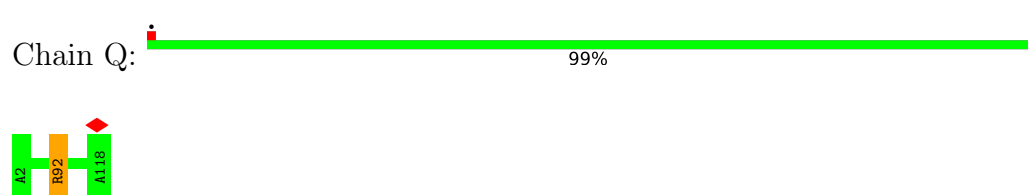
• Molecule 16: 50S ribosomal protein L18



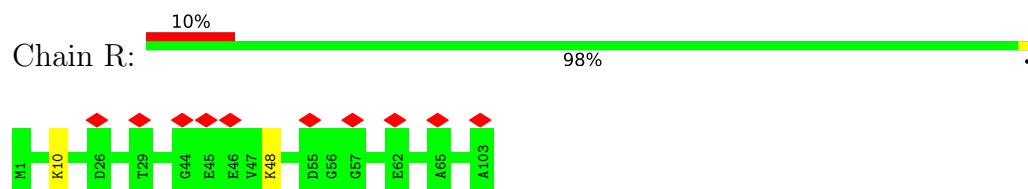
• Molecule 17: 50S ribosomal protein L19



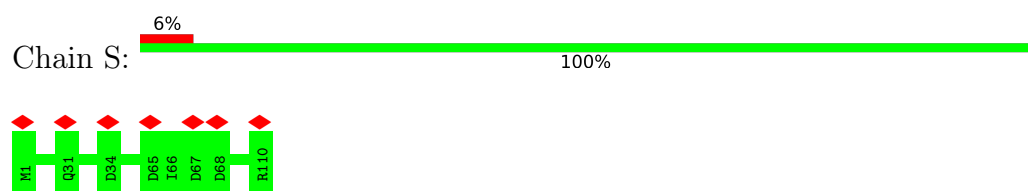
• Molecule 18: 50S ribosomal protein L20



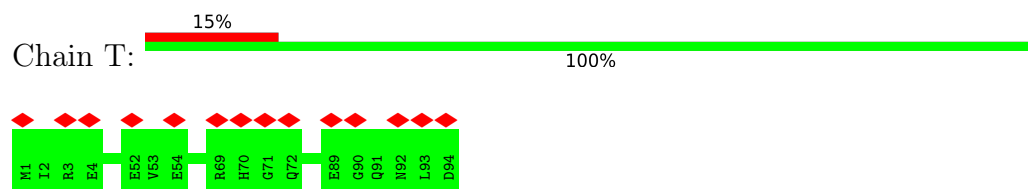
• Molecule 19: 50S ribosomal protein L21



• Molecule 20: 50S ribosomal protein L22

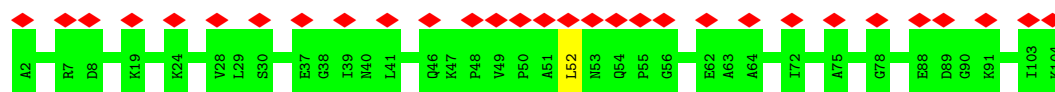


• Molecule 21: 50S ribosomal protein L23

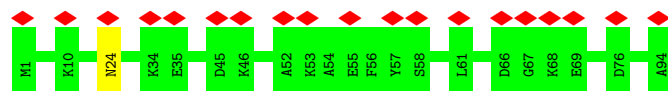


• Molecule 22: 50S ribosomal protein L24

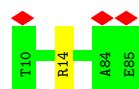




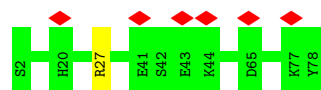
- Molecule 23: 50S ribosomal protein L25



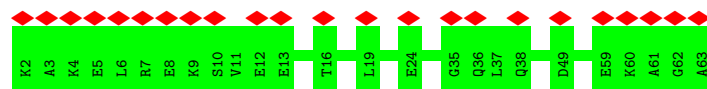
- Molecule 24: 50S ribosomal protein L27



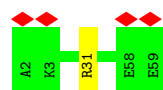
- Molecule 25: 50S ribosomal protein L28



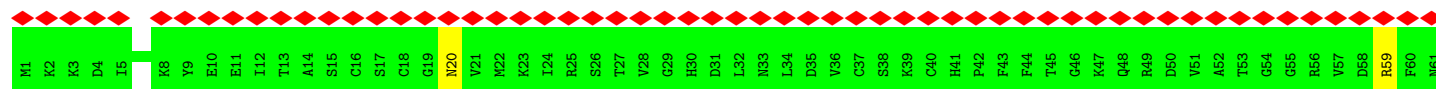
- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30

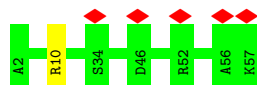


- Molecule 28: 50S ribosomal protein L31

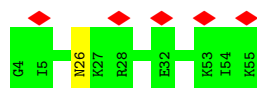




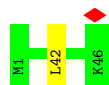
- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



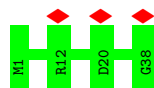
- Molecule 31: 50S ribosomal protein L34



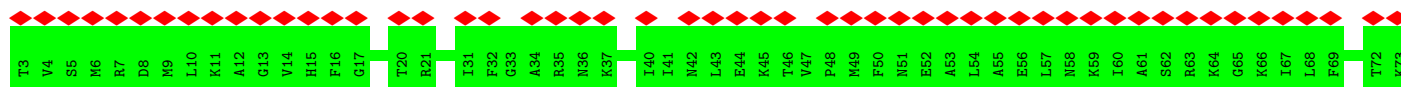
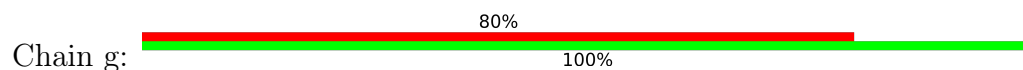
- Molecule 32: 50S ribosomal protein L35

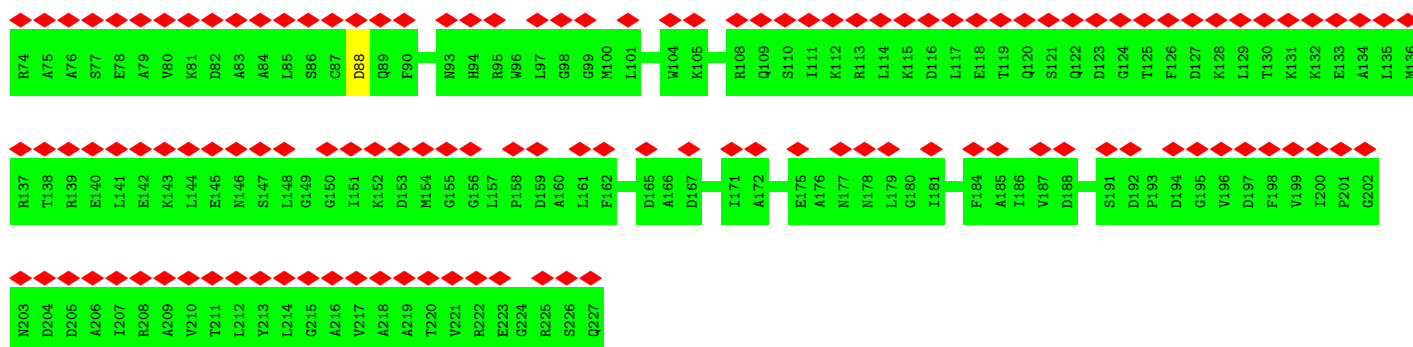


- Molecule 33: 50S ribosomal protein L36



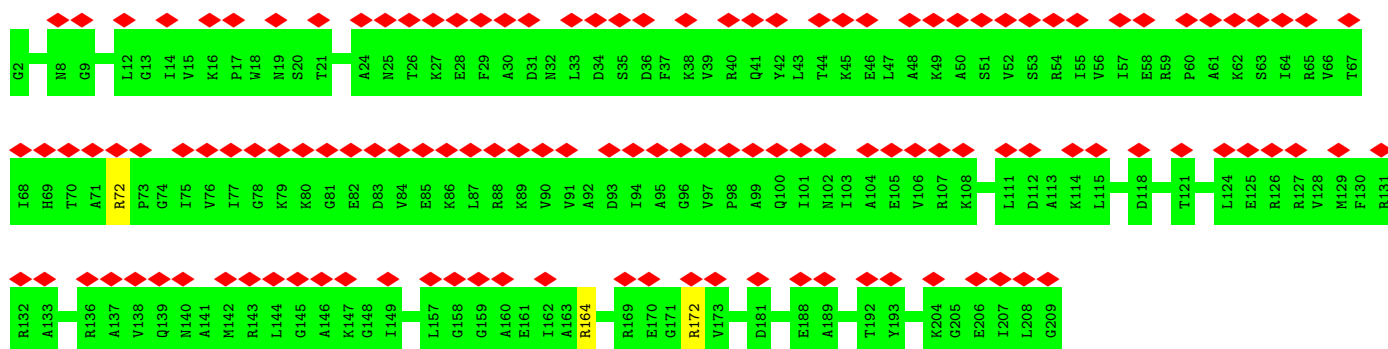
- Molecule 34: 30S ribosomal protein S2





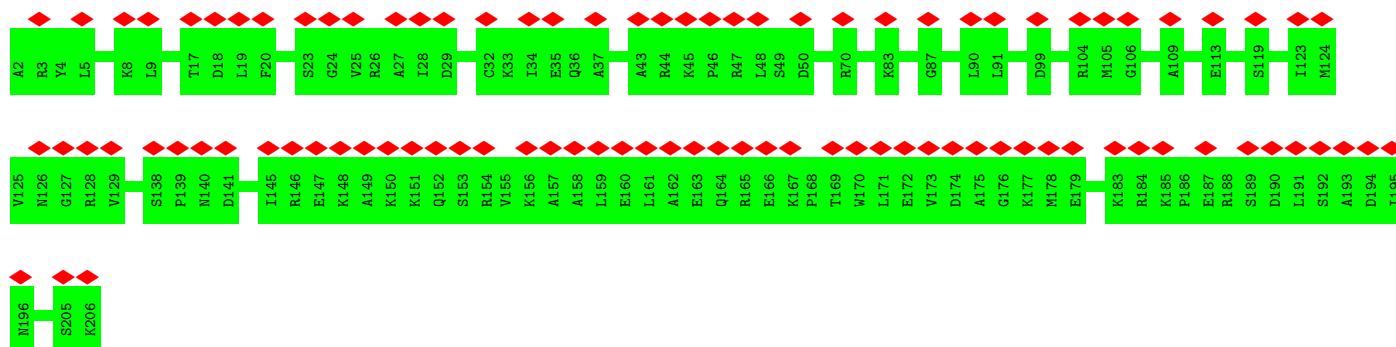
• Molecule 35: 30S ribosomal protein S3

Chain h: 61% 99%



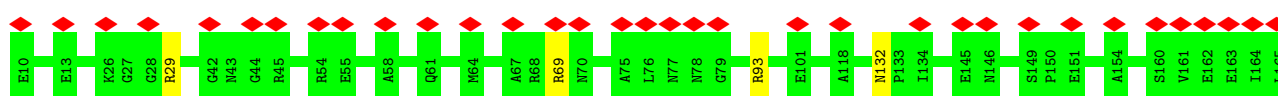
• Molecule 36: 30S ribosomal protein S4

Chain i: 46% 100%

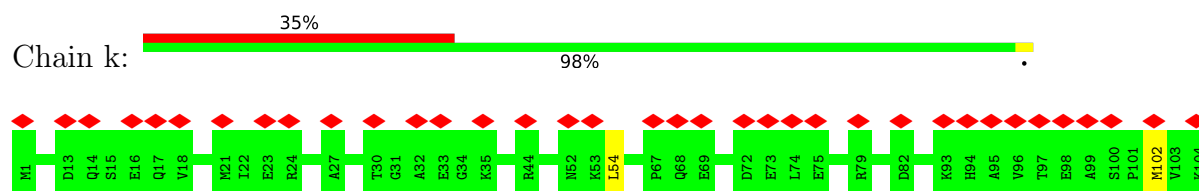


• Molecule 37: 30S ribosomal protein S5

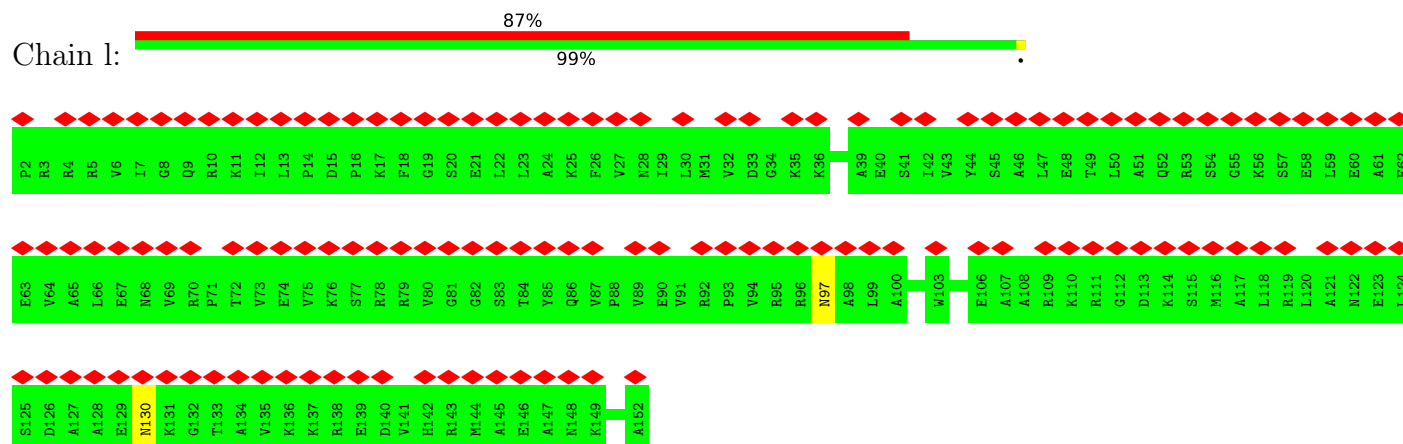
Chain j: 22% 97%



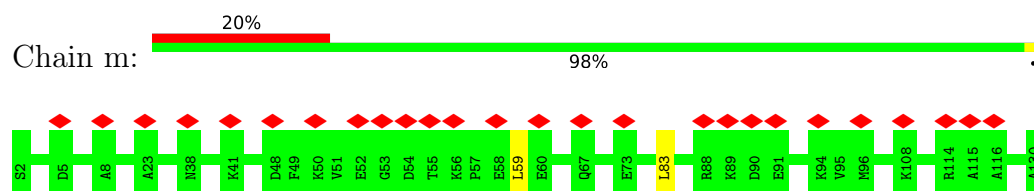
• Molecule 38: 30S ribosomal protein S6



• Molecule 39: 30S ribosomal protein S7

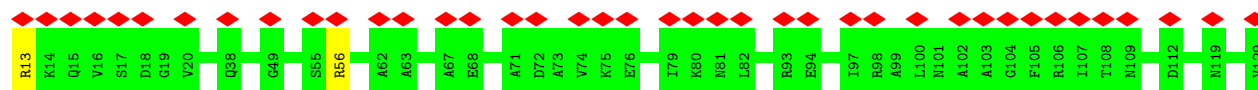


• Molecule 40: 30S ribosomal protein S8

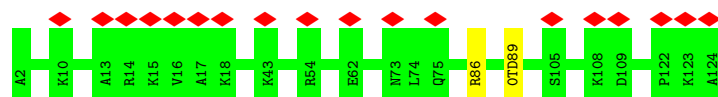




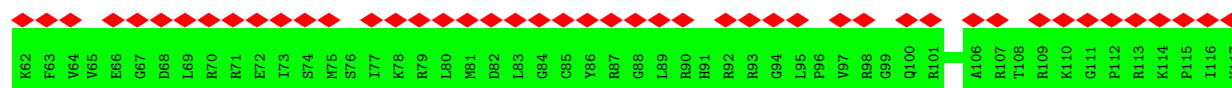
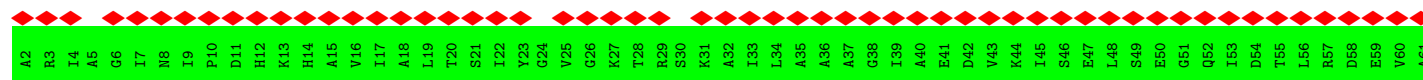
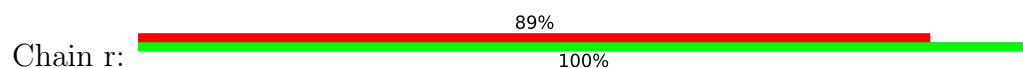
- Molecule 43: 30S ribosomal protein S11



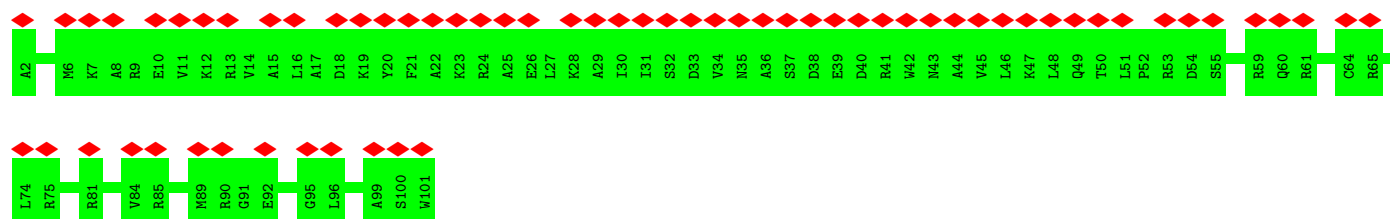
- Molecule 44: 30S ribosomal protein S12



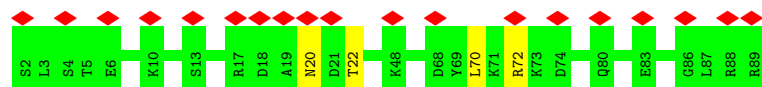
- Molecule 45: 30S ribosomal protein S13



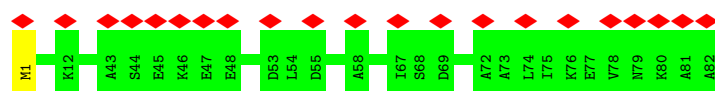
- Molecule 46: 30S ribosomal protein S14



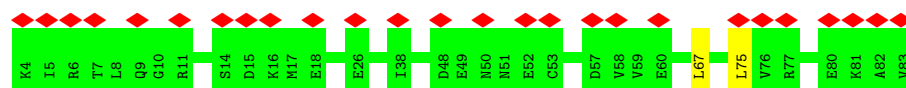
- Molecule 47: 30S ribosomal protein S15



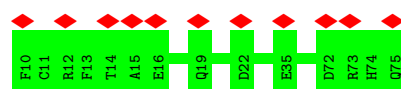
- Molecule 48: 30S ribosomal protein S16



- Molecule 49: 30S ribosomal protein S17



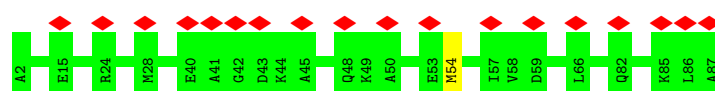
- Molecule 50: 30S ribosomal protein S18



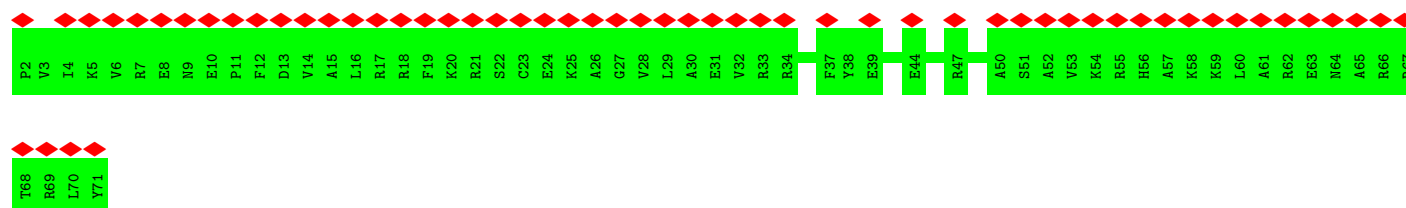
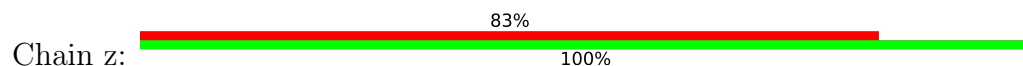
- Molecule 51: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94371	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.875	Depositor
Minimum map value	-0.602	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	392.19998, 392.19998, 392.19998	wwPDB
Map dimensions	370, 370, 370	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, G7M, 6MZ, 5MU, 2MA, 4OC, OMU, OMC, ZN, 1MG, MG, PSU, OMG, 3TD, 5MC, MA6, 0TD, UR3, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.93	3/106185 (0.0%)	1.13	561/165633 (0.3%)
2	3	0.73	0/2872	1.08	12/4478 (0.3%)
3	B	0.53	0/2122	0.68	1/2852 (0.0%)
4	C	0.50	0/1586	0.66	0/2134
5	D	0.44	0/1571	0.61	0/2113
6	E	0.34	0/1435	0.63	2/1926 (0.1%)
7	F	0.36	0/1333	0.60	0/1805
8	G	0.30	0/1122	0.62	1/1515 (0.1%)
9	H	0.35	0/993	0.72	2/1340 (0.1%)
10	I	0.31	0/998	0.63	0/1348
11	J	0.49	0/1152	0.59	0/1551
12	K	0.50	0/955	0.69	0/1279
13	L	0.47	1/1062 (0.1%)	0.69	0/1413
14	M	0.46	0/1093	0.64	0/1460
15	N	0.49	0/964	0.64	0/1289
16	O	0.37	0/902	0.62	0/1209
17	P	0.47	0/929	0.61	0/1242
18	Q	0.54	0/960	0.65	1/1278 (0.1%)
19	R	0.48	0/829	0.67	0/1107
20	S	0.47	0/864	0.62	0/1156
21	T	0.42	0/752	0.65	0/1005
22	U	0.40	0/796	0.59	1/1062 (0.1%)
23	V	0.41	0/766	0.58	0/1025
24	W	0.47	0/589	0.60	0/779
25	X	0.48	0/635	0.59	0/848
26	Y	0.33	0/502	0.61	0/667
27	Z	0.38	0/452	0.61	0/605
28	a	0.32	0/531	0.55	0/709
29	b	0.48	0/450	0.70	0/599
30	c	0.46	0/433	0.65	0/576
31	d	0.52	0/380	0.72	1/498 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.48	0/513	0.71	0/676
33	f	0.47	0/303	0.62	0/397
34	g	0.33	0/1791	0.61	1/2413 (0.0%)
35	h	0.33	0/1663	0.58	0/2241
36	i	0.35	0/1665	0.57	0/2227
37	j	0.43	0/1165	0.66	0/1568
38	k	0.38	0/867	0.62	0/1171
39	l	0.31	0/1195	0.61	0/1602
40	m	0.40	0/989	0.62	1/1326 (0.1%)
41	n	0.34	0/1034	0.67	0/1375
42	o	0.36	0/800	0.66	0/1082
43	p	0.39	0/893	0.56	0/1205
44	q	0.44	0/960	0.68	0/1286
45	r	0.30	0/909	0.66	0/1215
46	s	0.32	0/817	0.54	0/1088
47	t	0.38	0/722	0.59	0/964
48	u	0.38	0/659	0.62	0/884
49	v	0.38	0/658	0.67	2/881 (0.2%)
50	w	0.39	0/553	0.57	0/743
51	x	0.31	0/680	0.56	0/915
52	y	0.35	0/675	0.51	0/895
53	z	0.33	0/597	0.56	0/792
All	All	0.81	4/156321 (0.0%)	1.02	586/233447 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	39	0
3	B	0	2
10	I	0	1
12	K	0	1
32	e	0	1
38	k	0	1
All	All	39	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2393	U	C1'-N1	6.57	1.58	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	496	A	N9-C4	6.55	1.41	1.37
13	L	60	ARG	C-N	-5.20	1.22	1.34
1	1	1625	A	N9-C4	-5.12	1.34	1.37

All (586) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	467	U	C2-N1-C1'	11.57	131.59	117.70
1	1	1518	U	N3-C2-O2	-10.46	114.88	122.20
1	1	467	U	N1-C2-O2	10.30	130.01	122.80
1	1	2018	G	O4'-C1'-N9	10.21	116.37	108.20
1	1	1518	U	N1-C2-O2	9.83	129.68	122.80
1	1	328	C	N1-C2-O2	9.44	124.56	118.90
1	1	632	U	N3-C2-O2	-9.40	115.62	122.20
1	1	632	U	C2-N1-C1'	9.37	128.94	117.70
1	1	328	C	C2-N1-C1'	9.28	129.01	118.80
1	1	754	C	N1-C2-O2	9.24	124.44	118.90
1	1	2819	U	C2-N1-C1'	9.22	128.77	117.70
1	1	467	U	N3-C2-O2	-9.16	115.78	122.20
1	1	368	U	C2-N1-C1'	9.12	128.64	117.70
1	1	2547	G	N3-C4-N9	9.06	131.44	126.00
1	1	1518	U	C2-N1-C1'	9.04	128.55	117.70
1	1	632	U	N1-C2-O2	9.00	129.10	122.80
1	1	3909	C	N1-C2-O2	8.76	124.16	118.90
1	1	4091	U	N3-C2-O2	-8.72	116.10	122.20
1	1	368	U	N1-C2-O2	8.70	128.89	122.80
9	H	81	LEU	CA-CB-CG	8.63	135.15	115.30
1	1	2819	U	N1-C2-O2	8.58	128.80	122.80
1	1	4121	U	N3-C2-O2	-8.50	116.25	122.20
1	1	2505	U	N1-C2-O2	8.45	128.71	122.80
2	3	89	U	N1-C2-O2	8.39	128.68	122.80
1	1	754	C	C2-N1-C1'	8.38	128.01	118.80
1	1	3635	C	N1-C2-O2	8.29	123.87	118.90
1	1	1158	C	C2-N1-C1'	8.29	127.91	118.80
1	1	1644	U	C2-N1-C1'	8.24	127.59	117.70
1	1	2547	G	C4-N9-C1'	8.17	137.12	126.50
1	1	4222	C	N1-C2-O2	8.13	123.78	118.90
1	1	4121	U	N1-C2-O2	8.12	128.48	122.80
1	1	2547	G	N3-C4-C5	-8.10	124.55	128.60
2	3	89	U	N3-C2-O2	-8.09	116.54	122.20
1	1	1397	C	C2-N1-C1'	8.06	127.67	118.80
1	1	2820	C	N1-C2-O2	7.99	123.69	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	467	U	C6-N1-C1'	-7.99	110.02	121.20
1	1	2623	C	C6-N1-C2	-7.93	117.13	120.30
1	1	2819	U	N3-C2-O2	-7.93	116.65	122.20
1	1	439	U	N1-C2-O2	7.92	128.34	122.80
1	1	876	C	N1-C2-O2	7.90	123.64	118.90
1	1	2623	C	N1-C2-O2	7.90	123.64	118.90
1	1	1582	C	N1-C2-O2	7.88	123.63	118.90
1	1	3549	C	C6-N1-C2	-7.86	117.16	120.30
1	1	439	U	N3-C2-O2	-7.85	116.70	122.20
1	1	328	C	N3-C2-O2	-7.79	116.45	121.90
1	1	3145	C	N1-C2-O2	7.79	123.57	118.90
1	1	3426	C	C5-C6-N1	7.73	124.86	121.00
1	1	1158	C	N1-C2-O2	7.73	123.54	118.90
1	1	368	U	N3-C2-O2	-7.72	116.80	122.20
1	1	503	C	C6-N1-C2	-7.70	117.22	120.30
1	1	1644	U	N1-C2-O2	7.67	128.17	122.80
1	1	2505	U	N3-C2-O2	-7.66	116.84	122.20
1	1	1704	C	C6-N1-C2	-7.65	117.24	120.30
1	1	2175	G	C2-N3-C4	7.59	115.70	111.90
2	3	89	U	C2-N1-C1'	7.59	126.80	117.70
1	1	4152	C	C6-N1-C2	-7.58	117.27	120.30
1	1	439	U	C2-N1-C1'	7.57	126.79	117.70
1	1	4091	U	N1-C2-O2	7.53	128.07	122.80
1	1	3549	C	C5-C6-N1	7.53	124.76	121.00
1	1	1109	C	C3'-C2'-C1'	7.50	107.50	101.50
1	1	496	A	C2-N3-C4	7.49	114.34	110.60
1	1	3542	C	N1-C2-O2	7.49	123.39	118.90
1	1	4091	U	C6-N1-C2	-7.45	116.53	121.00
9	H	117	LEU	CA-CB-CG	7.42	132.36	115.30
1	1	4122	C	C6-N1-C2	-7.39	117.34	120.30
1	1	3090	U	N1-C2-O2	7.39	127.97	122.80
1	1	1397	C	N1-C2-O2	7.30	123.28	118.90
1	1	2885	U	C5-C6-N1	7.28	126.34	122.70
1	1	3426	C	C6-N1-C2	-7.25	117.40	120.30
1	1	2851	C	C6-N1-C2	-7.24	117.40	120.30
1	1	2050	C	N1-C2-O2	7.19	123.22	118.90
1	1	4091	U	C5-C6-N1	7.18	126.29	122.70
1	1	2186	C	C6-N1-C2	-7.17	117.43	120.30
1	1	3766	C	C6-N1-C2	-7.14	117.44	120.30
1	1	5	U	N1-C2-O2	7.13	127.79	122.80
1	1	876	C	N3-C2-O2	-7.10	116.93	121.90
1	1	3542	C	N3-C2-O2	-7.09	116.94	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	4142	C	N1-C2-O2	7.07	123.14	118.90
1	1	3280	C	N1-C2-O2	7.07	123.14	118.90
1	1	2623	C	C2-N1-C1'	7.05	126.56	118.80
1	1	3635	C	C6-N1-C2	-7.05	117.48	120.30
1	1	4085	C	N1-C2-O2	7.04	123.12	118.90
1	1	2820	C	C5-C6-N1	7.03	124.52	121.00
1	1	1322	C	C6-N1-C2	-7.02	117.49	120.30
3	B	130	LEU	CA-CB-CG	7.00	131.39	115.30
1	1	2421	C	N1-C2-O2	6.98	123.09	118.90
1	1	1364	U	C2-N1-C1'	6.97	126.06	117.70
1	1	2820	C	C2-N1-C1'	6.94	126.44	118.80
1	1	3635	C	C2-N1-C1'	6.94	126.43	118.80
1	1	1644	U	N3-C2-O2	-6.93	117.35	122.20
1	1	1745	C	N1-C2-O2	6.93	123.06	118.90
1	1	2585	C	N1-C2-O2	6.92	123.05	118.90
1	1	1603	C	C6-N1-C2	-6.91	117.53	120.30
1	1	2547	G	C8-N9-C1'	-6.91	118.01	127.00
1	1	503	C	C5-C6-N1	6.91	124.45	121.00
1	1	1461	G	P-O3'-C3'	6.90	127.98	119.70
1	1	3635	C	N3-C2-O2	-6.89	117.08	121.90
1	1	470	C	C5-C6-N1	6.88	124.44	121.00
1	1	3488	U	C5-C6-N1	6.87	126.14	122.70
1	1	5	U	N3-C2-O2	-6.87	117.39	122.20
1	1	536	C	C6-N1-C2	-6.86	117.56	120.30
1	1	1704	C	C5-C6-N1	6.86	124.43	121.00
1	1	2820	C	C6-N1-C2	-6.86	117.56	120.30
1	1	2585	C	N3-C2-O2	-6.85	117.11	121.90
1	1	3090	U	C2-N1-C1'	6.84	125.91	117.70
1	1	3150	C	N1-C2-O2	6.84	123.01	118.90
1	1	328	C	C6-N1-C1'	-6.82	112.62	120.80
1	1	1482	U	N3-C2-O2	-6.81	117.43	122.20
1	1	1070	U	N3-C2-O2	-6.80	117.44	122.20
1	1	1646	C	N3-C2-O2	-6.80	117.14	121.90
1	1	3551	C	C6-N1-C2	-6.80	117.58	120.30
1	1	2175	G	N3-C4-C5	-6.77	125.22	128.60
1	1	3274	C	C6-N1-C2	-6.74	117.61	120.30
1	1	2141	C	C6-N1-C2	-6.73	117.61	120.30
1	1	2623	C	N3-C2-O2	-6.71	117.21	121.90
1	1	54	C	N1-C2-O2	6.68	122.91	118.90
1	1	1159	U	C2-N1-C1'	6.68	125.71	117.70
1	1	1992	C	N3-C2-O2	-6.68	117.23	121.90
1	1	1621	C	C6-N1-C2	-6.67	117.63	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1646	C	N1-C2-O2	6.67	122.90	118.90
1	1	99	C	N3-C2-O2	-6.66	117.24	121.90
1	1	1987	G	O4'-C1'-N9	6.66	113.53	108.20
1	1	4058	OMU	P-O3'-C3'	6.64	127.67	119.70
1	1	1158	C	N3-C2-O2	-6.64	117.25	121.90
1	1	403	C	N1-C2-O2	6.63	122.88	118.90
1	1	1608	U	C2-N1-C1'	6.63	125.66	117.70
1	1	3578	C	C6-N1-C2	-6.62	117.65	120.30
1	1	1582	C	C6-N1-C2	-6.60	117.66	120.30
1	1	3578	C	N1-C2-O2	6.59	122.85	118.90
1	1	2322	C	C6-N1-C2	-6.58	117.67	120.30
1	1	545	C	C6-N1-C2	-6.58	117.67	120.30
1	1	3500	C	C6-N1-C2	-6.57	117.67	120.30
1	1	754	C	N3-C2-O2	-6.56	117.31	121.90
1	1	3488	U	N1-C2-O2	6.56	127.39	122.80
1	1	40	C	N1-C2-O2	6.56	122.83	118.90
1	1	99	C	N1-C2-O2	6.55	122.83	118.90
1	1	4086	PSU	P-O3'-C3'	6.55	127.56	119.70
1	1	2016	C	C6-N1-C2	-6.55	117.68	120.30
1	1	3909	C	N3-C2-O2	-6.55	117.32	121.90
1	1	3462	U	N3-C2-O2	-6.54	117.62	122.20
1	1	2289	A	C2-N3-C4	6.50	113.85	110.60
1	1	210	C	C2-N1-C1'	6.50	125.95	118.80
1	1	3886	C	C6-N1-C2	-6.49	117.70	120.30
1	1	1575	C	C6-N1-C2	-6.49	117.70	120.30
1	1	1992	C	N1-C2-O2	6.49	122.79	118.90
1	1	1463	U	N3-C2-O2	-6.49	117.66	122.20
1	1	1322	C	N3-C2-O2	-6.47	117.37	121.90
1	1	4152	C	C5-C6-N1	6.47	124.24	121.00
1	1	3473	C	N3-C2-O2	-6.46	117.38	121.90
1	1	2559	C	C6-N1-C2	-6.46	117.72	120.30
1	1	368	U	C6-N1-C1'	-6.45	112.17	121.20
1	1	2610	C	C5-C6-N1	6.45	124.22	121.00
1	1	1465	G	C4-N9-C1'	6.44	134.87	126.50
1	1	2318	C	C6-N1-C2	-6.43	117.73	120.30
1	1	3496	C	C6-N1-C2	-6.42	117.73	120.30
1	1	2071	C	C6-N1-C2	-6.42	117.73	120.30
1	1	2904	C	N1-C2-O2	6.42	122.75	118.90
1	1	3971	C	N1-C2-O2	6.41	122.74	118.90
1	1	3860	C	N1-C2-O2	6.40	122.74	118.90
1	1	1406	U	N3-C2-O2	-6.40	117.72	122.20
1	1	1910	A	P-O3'-C3'	6.37	127.34	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3322	C	N1-C2-O2	6.36	122.72	118.90
1	1	3667	C	N1-C2-O2	6.35	122.71	118.90
1	1	2868	C	C6-N1-C2	-6.33	117.77	120.30
1	1	3481	G	N3-C4-N9	6.33	129.79	126.00
1	1	2544	G	N3-C4-N9	-6.32	122.21	126.00
1	1	1522	C	C6-N1-C2	-6.32	117.77	120.30
1	1	385	C	C6-N1-C2	-6.30	117.78	120.30
1	1	163	C	N1-C2-O2	6.30	122.68	118.90
1	1	3860	C	C6-N1-C2	-6.29	117.78	120.30
1	1	2400	U	P-O3'-C3'	6.29	127.25	119.70
1	1	3090	U	N3-C2-O2	-6.29	117.80	122.20
1	1	2559	C	N1-C2-O2	6.28	122.67	118.90
1	1	1664	U	N1-C2-O2	6.27	127.19	122.80
1	1	1829	C	N1-C2-O2	6.26	122.65	118.90
1	1	2885	U	C6-N1-C2	-6.25	117.25	121.00
1	1	3659	C	C5-C6-N1	6.24	124.12	121.00
1	1	4236	C	C6-N1-C2	-6.23	117.81	120.30
1	1	2461	PSU	OP2-P-O3'	6.22	118.89	105.20
1	1	3602	C	N1-C2-O2	6.22	122.63	118.90
1	1	496	A	N3-C4-C5	-6.22	122.45	126.80
1	1	3473	C	N1-C2-O2	6.21	122.63	118.90
1	1	754	C	C6-N1-C1'	-6.20	113.36	120.80
1	1	1453	C	C2-N1-C1'	6.20	125.62	118.80
1	1	3732	C	N1-C2-O2	6.19	122.61	118.90
1	1	792	A	O4'-C1'-N9	6.18	113.15	108.20
1	1	1582	C	C5-C6-N1	6.18	124.09	121.00
1	1	2290	G	P-O3'-C3'	6.17	127.11	119.70
40	m	59	LEU	CA-CB-CG	6.15	129.45	115.30
1	1	1620	U	N3-C2-O2	-6.14	117.90	122.20
1	1	2156	C	C6-N1-C2	-6.13	117.85	120.30
1	1	215	C	N1-C2-O2	6.13	122.58	118.90
1	1	2549	C	C5-C4-N4	-6.13	115.91	120.20
1	1	3411	C	N1-C2-O2	6.12	122.57	118.90
1	1	3462	U	N1-C2-O2	6.12	127.09	122.80
1	1	2452	C	N1-C2-O2	6.12	122.57	118.90
1	1	1698	C	C6-N1-C2	-6.11	117.86	120.30
1	1	1468	C	C6-N1-C2	-6.11	117.86	120.30
2	3	71	C	N1-C2-O2	6.11	122.56	118.90
1	1	2621	G	O4'-C1'-N9	6.10	113.08	108.20
1	1	467	U	C5-C6-N1	6.09	125.75	122.70
1	1	1514	C	C6-N1-C2	-6.09	117.86	120.30
1	1	2967	C	N1-C2-O2	6.09	122.55	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1395	C	N1-C2-O2	6.08	122.55	118.90
1	1	470	C	C6-N1-C2	-6.08	117.87	120.30
1	1	54	C	N3-C2-O2	-6.07	117.65	121.90
1	1	3909	C	C6-N1-C2	-6.07	117.87	120.30
1	1	4086	PSU	OP2-P-O3'	6.06	118.53	105.20
1	1	2321	C	C6-N1-C2	-6.05	117.88	120.30
1	1	3931	A	P-O3'-C3'	6.03	126.93	119.70
1	1	2803	C	C6-N1-C2	-6.02	117.89	120.30
1	1	443	C	N1-C2-O2	6.02	122.51	118.90
1	1	3453	C	C6-N1-C2	-6.01	117.89	120.30
1	1	4091	U	C2-N1-C1'	6.01	124.92	117.70
1	1	1937	U	N3-C2-O2	-6.01	118.00	122.20
1	1	3971	C	N3-C2-O2	-6.01	117.70	121.90
1	1	1745	C	N3-C2-O2	-6.00	117.70	121.90
1	1	2492	C	C6-N1-C2	-6.00	117.90	120.30
1	1	643	C	C6-N1-C2	-5.99	117.90	120.30
1	1	3667	C	C6-N1-C2	-5.99	117.90	120.30
1	1	2512	C	C6-N1-C2	-5.99	117.91	120.30
1	1	1397	C	C6-N1-C2	-5.97	117.91	120.30
1	1	3529	C	C6-N1-C2	-5.96	117.92	120.30
1	1	4111	PSU	OP2-P-O3'	5.96	118.30	105.20
1	1	3145	C	N3-C2-O2	-5.94	117.74	121.90
1	1	3162	C	C6-N1-C2	-5.94	117.92	120.30
1	1	1664	U	N3-C2-O2	-5.94	118.04	122.20
1	1	496	A	N3-C4-N9	5.94	132.15	127.40
1	1	1364	U	N1-C2-O2	5.94	126.96	122.80
1	1	1070	U	N1-C2-O2	5.93	126.95	122.80
1	1	1620	U	N1-C2-O2	5.91	126.94	122.80
1	1	4151	G	O4'-C1'-N9	5.91	112.92	108.20
1	1	3281	U	N3-C2-O2	-5.91	118.07	122.20
1	1	1322	C	C2-N1-C1'	5.90	125.29	118.80
1	1	403	C	C6-N1-C2	-5.90	117.94	120.30
1	1	1664	U	C2-N1-C1'	5.90	124.78	117.70
1	1	4383	C	C6-N1-C2	-5.90	117.94	120.30
1	1	3549	C	N1-C2-O2	5.89	122.44	118.90
1	1	156	C	C6-N1-C2	-5.89	117.94	120.30
1	1	3385	C	C6-N1-C2	-5.88	117.95	120.30
1	1	2421	C	N3-C2-O2	-5.88	117.78	121.90
1	1	403	C	N3-C2-O2	-5.88	117.78	121.90
1	1	311	C	C6-N1-C2	-5.88	117.95	120.30
1	1	1950	C	C6-N1-C2	-5.88	117.95	120.30
1	1	632	U	C6-N1-C1'	-5.87	112.98	121.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1364	U	N3-C2-O2	-5.87	118.09	122.20
1	1	1159	U	N1-C2-O2	5.87	126.91	122.80
1	1	1849	C	N1-C2-O2	5.87	122.42	118.90
1	1	2606	C	C6-N1-C2	-5.87	117.95	120.30
1	1	736	C	C6-N1-C2	-5.86	117.96	120.30
1	1	1478	C	N1-C2-O2	5.86	122.41	118.90
1	1	2050	C	N3-C2-O2	-5.85	117.80	121.90
1	1	4280	C	C6-N1-C2	-5.84	117.96	120.30
1	1	4426	C	C6-N1-C2	-5.84	117.96	120.30
1	1	4142	C	N3-C2-O2	-5.84	117.81	121.90
1	1	2193	C	N3-C2-O2	-5.84	117.81	121.90
1	1	1582	C	N3-C2-O2	-5.83	117.82	121.90
1	1	2497	C	C6-N1-C2	-5.83	117.97	120.30
1	1	1397	C	N3-C2-O2	-5.83	117.82	121.90
1	1	2846	U	C2-N1-C1'	5.83	124.69	117.70
1	1	2471	C	C6-N1-C2	-5.82	117.97	120.30
1	1	2885	U	P-O3'-C3'	5.82	126.69	119.70
1	1	4278	C	C6-N1-C2	-5.82	117.97	120.30
1	1	1158	C	C6-N1-C1'	-5.82	113.81	120.80
6	E	174	ASP	CB-CG-OD1	5.82	123.54	118.30
1	1	3963	PSU	P-O3'-C3'	5.82	126.68	119.70
1	1	2819	U	C6-N1-C1'	-5.82	113.06	121.20
1	1	2804	C	C6-N1-C2	-5.81	117.97	120.30
1	1	2318	C	N1-C2-O2	5.81	122.39	118.90
1	1	1465	G	C8-N9-C1'	-5.81	119.45	127.00
1	1	2820	C	N3-C2-O2	-5.80	117.84	121.90
1	1	496	A	C8-N9-C4	-5.80	103.48	105.80
2	3	89	U	C5-C6-N1	5.79	125.60	122.70
2	3	91	C	C6-N1-C2	-5.79	117.98	120.30
1	1	1644	U	C6-N1-C1'	-5.78	113.11	121.20
31	d	42	LEU	CA-CB-CG	5.78	128.60	115.30
1	1	2323	C	C6-N1-C2	-5.78	117.99	120.30
1	1	3328	C	C6-N1-C2	-5.77	117.99	120.30
1	1	3578	C	N3-C2-O2	-5.77	117.86	121.90
1	1	2175	G	N3-C4-N9	5.77	129.46	126.00
1	1	2900	U	C6-N1-C1'	5.76	129.27	121.20
1	1	178	C	C6-N1-C2	-5.75	118.00	120.30
1	1	58	C	C6-N1-C2	-5.75	118.00	120.30
1	1	2016	C	N1-C2-O2	5.75	122.35	118.90
1	1	215	C	N3-C2-O2	-5.74	117.88	121.90
1	1	4245	U	N1-C2-O2	5.74	126.81	122.80
1	1	4245	U	N3-C2-O2	-5.73	118.19	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3659	C	C6-N1-C2	-5.73	118.01	120.30
1	1	210	C	N1-C2-O2	5.72	122.33	118.90
1	1	2193	C	C6-N1-C2	-5.72	118.01	120.30
1	1	3342	C	C6-N1-C2	-5.72	118.01	120.30
1	1	972	C	C6-N1-C2	-5.71	118.01	120.30
1	1	3488	U	N3-C2-O2	-5.70	118.21	122.20
1	1	3962	C	C6-N1-C2	-5.69	118.02	120.30
1	1	2836	C	N3-C2-O2	-5.69	117.92	121.90
1	1	1388	C	C6-N1-C2	-5.69	118.03	120.30
1	1	2243	C	C6-N1-C2	-5.68	118.03	120.30
1	1	2819	U	C5-C6-N1	5.68	125.54	122.70
1	1	2140	C	C6-N1-C2	-5.68	118.03	120.30
1	1	365	U	C2-N1-C1'	5.68	124.51	117.70
1	1	2882	C	N1-C2-O2	5.67	122.30	118.90
1	1	392	C	N1-C2-O2	5.66	122.30	118.90
1	1	2296	U	C5-C6-N1	-5.66	119.87	122.70
1	1	2836	C	N1-C2-O2	5.66	122.29	118.90
1	1	4229	C	C6-N1-C2	-5.65	118.04	120.30
1	1	2904	C	N3-C2-O2	-5.65	117.95	121.90
1	1	3818	U	C5-C6-N1	5.64	125.52	122.70
1	1	3280	C	N3-C2-O2	-5.64	117.95	121.90
1	1	1622	C	N3-C2-O2	-5.63	117.96	121.90
1	1	4222	C	N3-C2-O2	-5.63	117.96	121.90
1	1	3550	C	N1-C2-O2	5.62	122.27	118.90
1	1	400	C	C6-N1-C2	-5.61	118.05	120.30
1	1	316	C	C6-N1-C2	-5.61	118.06	120.30
1	1	2418	C	C6-N1-C2	-5.61	118.06	120.30
1	1	2585	C	C6-N1-C2	-5.61	118.06	120.30
1	1	2624	C	C6-N1-C2	-5.60	118.06	120.30
1	1	3770	C	N1-C2-O2	5.60	122.26	118.90
1	1	1463	U	N1-C2-O2	5.60	126.72	122.80
1	1	2623	C	C5-C6-N1	5.60	123.80	121.00
1	1	3643	U	C5-C6-N1	5.60	125.50	122.70
1	1	436	C	C6-N1-C2	-5.60	118.06	120.30
1	1	1646	C	C6-N1-C2	-5.60	118.06	120.30
1	1	2527	A	C2-N3-C4	5.59	113.40	110.60
1	1	1478	C	C6-N1-C2	-5.59	118.06	120.30
1	1	2318	C	C5-C6-N1	5.59	123.80	121.00
1	1	813	U	N3-C2-O2	-5.59	118.29	122.20
1	1	679	C	C6-N1-C2	-5.58	118.07	120.30
1	1	3150	C	C6-N1-C2	-5.58	118.07	120.30
1	1	4085	C	N3-C2-O2	-5.58	117.99	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3015	A	O4'-C1'-N9	5.58	112.66	108.20
1	1	2318	C	N3-C2-O2	-5.58	118.00	121.90
1	1	1889	C	N3-C2-O2	-5.58	118.00	121.90
1	1	2836	C	C6-N1-C2	-5.58	118.07	120.30
1	1	2264	C	N1-C2-O2	5.58	122.25	118.90
34	g	88	ASP	CB-CG-OD1	5.58	123.32	118.30
1	1	3897	G	O4'-C1'-N9	5.57	112.66	108.20
1	1	1518	U	C6-N1-C1'	-5.57	113.40	121.20
1	1	438	U	O4'-C1'-N1	5.57	112.65	108.20
1	1	525	C	C5-C6-N1	5.57	123.78	121.00
1	1	4258	C	C6-N1-C2	-5.57	118.07	120.30
1	1	3181	C	C6-N1-C2	-5.56	118.08	120.30
1	1	972	C	N1-C2-O2	5.56	122.24	118.90
1	1	2490	A	O4'-C1'-N9	5.55	112.64	108.20
1	1	436	C	N1-C2-O2	5.55	122.23	118.90
1	1	496	A	N7-C8-N9	5.55	116.58	113.80
1	1	3635	C	C5-C6-N1	5.55	123.78	121.00
1	1	2208	U	N1-C2-O2	5.54	126.68	122.80
1	1	1585	C	C6-N1-C2	-5.54	118.08	120.30
1	1	4085	C	C6-N1-C2	-5.54	118.08	120.30
1	1	4450	A	C2-N3-C4	5.53	113.37	110.60
1	1	536	C	C5-C6-N1	5.52	123.76	121.00
1	1	3301	C	C6-N1-C2	-5.51	118.09	120.30
1	1	3579	C	N1-C2-O2	5.51	122.21	118.90
2	3	90	C	C6-N1-C2	-5.51	118.10	120.30
1	1	2904	C	C6-N1-C2	-5.50	118.10	120.30
1	1	3285	U	C5-C6-N1	-5.50	119.95	122.70
1	1	2471	C	C5-C6-N1	5.50	123.75	121.00
1	1	3440	C	N3-C2-O2	-5.50	118.05	121.90
1	1	3971	C	C6-N1-C2	-5.50	118.10	120.30
1	1	940	C	C6-N1-C2	-5.50	118.10	120.30
1	1	3739	U	N1-C2-O2	5.50	126.65	122.80
1	1	2292	C	N1-C2-O2	5.49	122.19	118.90
1	1	1621	C	C5-C6-N1	5.48	123.74	121.00
1	1	3669	A	O5'-P-OP1	-5.48	100.77	105.70
1	1	4261	C	N1-C2-O2	5.48	122.19	118.90
1	1	235	C	N1-C2-O2	5.48	122.19	118.90
1	1	2470	C	C6-N1-C2	-5.48	118.11	120.30
1	1	1203	C	C6-N1-C2	-5.47	118.11	120.30
1	1	1457	A	C2-N3-C4	5.47	113.34	110.60
1	1	4252	U	C5-C6-N1	5.47	125.44	122.70
1	1	1406	U	N1-C2-O2	5.47	126.63	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3643	U	N1-C2-O2	5.47	126.63	122.80
1	1	1993	C	N3-C2-O2	-5.46	118.08	121.90
1	1	2943	C	N1-C2-O2	5.46	122.18	118.90
1	1	3909	C	C5-C6-N1	5.46	123.73	121.00
1	1	2070	C	C6-N1-C2	-5.46	118.12	120.30
1	1	764	C	N1-C2-O2	5.45	122.17	118.90
1	1	4112	C	C6-N1-C2	-5.45	118.12	120.30
1	1	993	G	C4-N9-C1'	5.45	133.59	126.50
1	1	2235	G	C4-N9-C1'	5.45	133.59	126.50
1	1	2452	C	N3-C2-O2	-5.45	118.09	121.90
49	v	75	LEU	CA-CB-CG	5.45	127.83	115.30
1	1	570	G	N3-C4-N9	5.45	129.27	126.00
1	1	1535	U	C5-C6-N1	5.45	125.42	122.70
1	1	3280	C	C5-C6-N1	5.44	123.72	121.00
1	1	2667	C	C6-N1-C2	-5.43	118.13	120.30
1	1	3949	C	C6-N1-C2	-5.43	118.13	120.30
1	1	1839	G	C4-N9-C1'	5.43	133.56	126.50
1	1	2016	C	C2-N1-C1'	5.43	124.77	118.80
1	1	3280	C	C6-N1-C2	-5.43	118.13	120.30
1	1	2627	C	C6-N1-C2	-5.43	118.13	120.30
1	1	4097	C	C6-N1-C2	-5.43	118.13	120.30
1	1	2901	A	O4'-C1'-N9	5.43	112.54	108.20
1	1	4209	C	C6-N1-C2	-5.43	118.13	120.30
1	1	1889	C	N1-C2-O2	5.42	122.16	118.90
1	1	222	C	C6-N1-C2	-5.42	118.13	120.30
1	1	2606	C	N1-C2-O2	5.42	122.15	118.90
1	1	1397	C	C5-C6-N1	5.42	123.71	121.00
1	1	1717	C	C6-N1-C2	-5.42	118.13	120.30
1	1	3150	C	N3-C2-O2	-5.42	118.11	121.90
1	1	3667	C	N3-C2-O2	-5.42	118.11	121.90
1	1	2271	C	N1-C2-O2	5.41	122.15	118.90
1	1	178	C	C5-C6-N1	5.41	123.70	121.00
1	1	1298	U	N3-C2-O2	-5.40	118.42	122.20
1	1	1608	U	N1-C2-O2	5.40	126.58	122.80
1	1	620	C	N1-C2-O2	5.39	122.14	118.90
1	1	4261	C	C2-N1-C1'	5.39	124.73	118.80
1	1	1389	C	N1-C2-O2	5.39	122.13	118.90
1	1	485	U	N1-C2-O2	5.39	126.57	122.80
1	1	1582	C	C2-N1-C1'	5.39	124.72	118.80
1	1	4100	C	C6-N1-C2	-5.38	118.15	120.30
1	1	3512	C	N1-C2-O2	5.38	122.13	118.90
1	1	4152	C	N1-C2-O2	5.38	122.13	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3980	U	N3-C2-O2	-5.38	118.44	122.20
1	1	3732	C	N3-C2-O2	-5.38	118.14	121.90
22	U	52	LEU	CA-CB-CG	5.37	127.66	115.30
1	1	924	C	C6-N1-C2	-5.37	118.15	120.30
1	1	2344	C	N1-C2-O2	5.37	122.12	118.90
1	1	2208	U	N3-C2-O2	-5.37	118.44	122.20
1	1	1279	G	C4-N9-C1'	5.36	133.47	126.50
1	1	3980	U	N1-C2-O2	5.35	126.55	122.80
1	1	3767	C	C6-N1-C2	-5.35	118.16	120.30
1	1	2352	U	C2-N1-C1'	5.34	124.11	117.70
1	1	2846	U	N3-C2-O2	-5.34	118.46	122.20
1	1	485	U	C2-N1-C1'	5.34	124.11	117.70
1	1	526	C	C6-N1-C2	-5.34	118.16	120.30
1	1	3443	A	O4'-C1'-N9	5.34	112.47	108.20
6	E	123	ASP	CB-CG-OD1	5.34	123.11	118.30
1	1	3471	C	O5'-P-OP2	-5.33	100.90	105.70
1	1	3868	C	C6-N1-C2	-5.33	118.17	120.30
1	1	2130	C	C6-N1-C2	-5.33	118.17	120.30
1	1	3053	C	N1-C2-O2	5.33	122.09	118.90
1	1	3860	C	N3-C2-O2	-5.32	118.18	121.90
1	1	469	C	N1-C2-O2	5.32	122.09	118.90
1	1	1397	C	C6-N1-C1'	-5.32	114.42	120.80
1	1	1715	C	C6-N1-C2	-5.31	118.17	120.30
1	1	3176	C	C5-C6-N1	5.31	123.66	121.00
1	1	3464	C	C6-N1-C2	-5.31	118.18	120.30
1	1	4	U	C2-N1-C1'	5.30	124.06	117.70
1	1	1829	C	C2-N1-C1'	5.30	124.63	118.80
1	1	2289	A	C4-N9-C1'	5.30	135.84	126.30
1	1	1114	C	N3-C2-O2	-5.30	118.19	121.90
1	1	4012	U	O4'-C1'-N1	5.30	112.44	108.20
1	1	556	C	C6-N1-C2	-5.30	118.18	120.30
1	1	2851	C	C5-C6-N1	5.30	123.65	121.00
2	3	30	C	C6-N1-C2	-5.29	118.18	120.30
1	1	2353	U	N3-C2-O2	-5.29	118.50	122.20
1	1	3150	C	C2-N1-C1'	5.29	124.62	118.80
1	1	4068	U	N3-C2-O2	-5.29	118.50	122.20
1	1	2246	C	N1-C2-O2	5.29	122.07	118.90
1	1	2453	A	N1-C2-N3	-5.28	126.66	129.30
1	1	2504	C	N1-C2-O2	5.28	122.07	118.90
1	1	2855	C	C6-N1-C2	-5.27	118.19	120.30
1	1	2292	C	N3-C2-O2	-5.27	118.21	121.90
2	3	91	C	N1-C2-O2	5.26	122.06	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	882	C	N1-C2-O2	5.26	122.06	118.90
1	1	1990	C	N1-C2-O2	5.26	122.06	118.90
1	1	1002	G	C4-N9-C1'	5.26	133.34	126.50
1	1	3578	C	C5-C6-N1	5.26	123.63	121.00
1	1	4068	U	N1-C2-O2	5.26	126.48	122.80
1	1	564	C	C6-N1-C2	-5.25	118.20	120.30
1	1	1395	C	C2-N1-C1'	5.25	124.58	118.80
1	1	1591	G	O5'-P-OP2	-5.25	100.97	105.70
1	1	1839	G	N3-C4-C5	-5.25	125.97	128.60
1	1	2854	C	N1-C2-O2	5.24	122.05	118.90
1	1	221	C	N1-C2-O2	5.24	122.04	118.90
1	1	370	C	C6-N1-C2	-5.24	118.20	120.30
1	1	3197	C	C6-N1-C2	-5.24	118.20	120.30
8	G	12	LEU	CA-CB-CG	5.24	127.35	115.30
1	1	52	C	C6-N1-C2	-5.24	118.20	120.30
1	1	1427	C	C6-N1-C2	-5.23	118.21	120.30
1	1	2610	C	C2-N1-C1'	5.23	124.55	118.80
1	1	1612	C	C6-N1-C2	-5.23	118.21	120.30
1	1	2559	C	N3-C2-O2	-5.23	118.24	121.90
1	1	4279	C	C6-N1-C2	-5.23	118.21	120.30
2	3	89	U	C6-N1-C2	-5.23	117.86	121.00
1	1	2343	C	C6-N1-C2	-5.22	118.21	120.30
1	1	3728	C	C6-N1-C2	-5.22	118.21	120.30
1	1	2547	G	N7-C8-N9	5.22	115.71	113.10
1	1	2254	G	O4'-C1'-N9	5.21	112.36	108.20
1	1	3860	C	C5-C6-N1	5.21	123.60	121.00
1	1	2969	C	C6-N1-C2	-5.21	118.22	120.30
1	1	1114	C	N1-C2-O2	5.20	122.02	118.90
1	1	3290	A	N9-C4-C5	-5.20	103.72	105.80
1	1	2497	C	C5-C6-N1	5.20	123.60	121.00
1	1	3512	C	C6-N1-C2	-5.20	118.22	120.30
1	1	436	C	C2-N1-C1'	5.20	124.52	118.80
49	v	67	LEU	CA-CB-CG	5.20	127.25	115.30
1	1	4440	C	C6-N1-C2	-5.20	118.22	120.30
1	1	1118	U	N1-C2-O2	5.19	126.43	122.80
1	1	1611	C	C6-N1-C2	-5.19	118.22	120.30
1	1	2258	A	C5-N7-C8	-5.18	101.31	103.90
1	1	3440	C	C6-N1-C2	-5.18	118.23	120.30
1	1	1876	G	O4'-C1'-N9	-5.18	104.06	108.20
1	1	2967	C	N3-C2-O2	-5.18	118.28	121.90
1	1	3756	G	N3-C4-C5	-5.18	126.01	128.60
1	1	4312	C	N3-C2-O2	-5.18	118.28	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	392	C	N3-C2-O2	-5.17	118.28	121.90
1	1	3039	C	N1-C2-O2	5.17	122.00	118.90
1	1	1745	C	C2-N1-C1'	5.17	124.49	118.80
1	1	4312	C	C6-N1-C2	-5.17	118.23	120.30
1	1	972	C	N3-C2-O2	-5.17	118.28	121.90
1	1	2242	C	C6-N1-C2	-5.17	118.23	120.30
1	1	492	C	C6-N1-C2	-5.17	118.23	120.30
1	1	1159	U	N3-C2-O2	-5.16	118.59	122.20
1	1	2264	C	N3-C2-O2	-5.16	118.29	121.90
2	3	97	C	C6-N1-C2	-5.16	118.24	120.30
1	1	3969	C	C6-N1-C2	-5.15	118.24	120.30
1	1	4087	G	O4'-C1'-N9	5.15	112.32	108.20
1	1	1482	U	N1-C2-O2	5.15	126.41	122.80
1	1	1001	C	N1-C2-O2	5.15	121.99	118.90
1	1	2504	C	N3-C2-O2	-5.15	118.30	121.90
1	1	2830	G	O4'-C1'-N9	5.15	112.32	108.20
1	1	488	C	C6-N1-C2	-5.14	118.24	120.30
1	1	3896	U	N3-C2-O2	-5.14	118.60	122.20
1	1	2193	C	N1-C2-O2	5.14	121.98	118.90
1	1	2547	G	C2-N3-C4	5.14	114.47	111.90
1	1	1572	C	N1-C2-O2	5.14	121.98	118.90
1	1	2016	C	N3-C2-O2	-5.14	118.30	121.90
1	1	222	C	N3-C2-O2	-5.14	118.31	121.90
1	1	1849	C	C6-N1-C2	-5.14	118.25	120.30
1	1	264	C	C6-N1-C2	-5.13	118.25	120.30
1	1	1537	C	C6-N1-C2	-5.13	118.25	120.30
1	1	3282	G	C4-N9-C1'	5.13	133.17	126.50
1	1	1158	C	C6-N1-C2	-5.13	118.25	120.30
1	1	3053	C	N3-C2-O2	-5.12	118.31	121.90
1	1	3423	PSU	P-O3'-C3'	5.12	125.85	119.70
1	1	1322	C	N1-C2-O2	5.12	121.97	118.90
1	1	485	U	N3-C2-O2	-5.12	118.62	122.20
1	1	2869	C	N3-C2-O2	-5.12	118.32	121.90
1	1	222	C	N1-C2-O2	5.12	121.97	118.90
1	1	3322	C	N3-C2-O2	-5.12	118.32	121.90
1	1	4012	U	C2-N1-C1'	-5.11	111.56	117.70
1	1	764	C	N3-C2-O2	-5.11	118.32	121.90
1	1	2051	U	C2-N1-C1'	5.11	123.83	117.70
1	1	3232	C	N1-C2-O2	5.11	121.96	118.90
1	1	1522	C	N1-C2-O2	5.10	121.96	118.90
1	1	2471	C	N1-C2-O2	5.10	121.96	118.90
1	1	5	U	C2-N1-C1'	5.10	123.82	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2493	C	C6-N1-C2	-5.10	118.26	120.30
1	1	4021	C	C6-N1-C2	-5.10	118.26	120.30
1	1	108	G	C6-C5-N7	-5.10	127.34	130.40
1	1	1069	C	C6-N1-C2	-5.10	118.26	120.30
1	1	3281	U	N1-C2-O2	5.10	126.37	122.80
1	1	3579	C	N3-C2-O2	-5.09	118.33	121.90
1	1	2290	G	OP1-P-O3'	5.09	116.40	105.20
1	1	1060	U	N1-C2-O2	5.09	126.36	122.80
1	1	4229	C	C5-C6-N1	5.09	123.55	121.00
1	1	4	U	N3-C2-O2	-5.09	118.64	122.20
1	1	1395	C	C6-N1-C2	-5.09	118.27	120.30
1	1	2511	C	N1-C2-O2	5.09	121.95	118.90
1	1	352	C	C6-N1-C2	-5.08	118.27	120.30
1	1	1395	C	N3-C2-O2	-5.08	118.34	121.90
1	1	916	U	N1-C2-O2	5.08	126.35	122.80
1	1	1759	C	C6-N1-C2	-5.07	118.27	120.30
1	1	1443	C	C6-N1-C2	-5.07	118.27	120.30
1	1	2882	C	C6-N1-C2	-5.07	118.27	120.30
1	1	1557	G	N3-C4-C5	-5.06	126.07	128.60
1	1	1711	G	O4'-C1'-N9	5.05	112.24	108.20
1	1	2289	A	N3-C4-N9	5.05	131.44	127.40
1	1	2632	A	C8-N9-C4	-5.05	103.78	105.80
1	1	1518	U	C6-N1-C2	-5.05	117.97	121.00
1	1	2513	C	C6-N1-C2	-5.05	118.28	120.30
1	1	3579	C	C6-N1-C2	-5.05	118.28	120.30
1	1	2624	C	C5-C6-N1	5.04	123.52	121.00
1	1	4266	C	C6-N1-C2	-5.04	118.28	120.30
1	1	1899	C	C6-N1-C2	-5.04	118.28	120.30
1	1	2882	C	N3-C2-O2	-5.04	118.37	121.90
1	1	3328	C	N3-C2-O2	-5.04	118.38	121.90
1	1	4378	C	C6-N1-C2	-5.04	118.29	120.30
1	1	4164	C	C6-N1-C2	-5.03	118.29	120.30
18	Q	92	ARG	CA-CB-CG	5.03	124.47	113.40
1	1	3699	G	C4-C5-N7	5.03	112.81	110.80
1	1	1620	U	C2-N1-C1'	5.03	123.73	117.70
1	1	3267	C	C6-N1-C2	-5.03	118.29	120.30
1	1	4095	A	N1-C2-N3	-5.02	126.79	129.30
1	1	1635	C	C6-N1-C2	-5.02	118.29	120.30
1	1	4155	C	N1-C2-O2	5.02	121.91	118.90
1	1	2559	C	C5-C6-N1	5.02	123.51	121.00
1	1	153	C	C6-N1-C2	-5.01	118.29	120.30
1	1	3553	C	N1-C2-O2	5.01	121.91	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1462	U	C5-C6-N1	5.01	125.20	122.70
1	1	910	C	C6-N1-C2	-5.00	118.30	120.30
2	3	17	C	C6-N1-C2	-5.00	118.30	120.30
1	1	2344	C	N3-C2-O2	-5.00	118.40	121.90
1	1	2421	C	C6-N1-C2	-5.00	118.30	120.30

All (39) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	516	PSU	C3',C4'
1	1	527	7MG	C3'
1	1	1402	4OC	C1',C3'
1	1	2251	1MG	C2',C1'
1	1	2252	PSU	C3',C4'
1	1	2253	5MU	C2',C4'
1	1	2461	PSU	C3',C4'
1	1	3124	6MZ	C2',C3'
1	1	3417	PSU	C3',C4'
1	1	3421	3TD	C3'
1	1	3423	PSU	C3',C4'
1	1	3445	5MU	C2',C4'
1	1	3536	6MZ	C2',C3'
1	1	3575	G7M	C2'
1	1	3757	OMG	C2'
1	1	3963	PSU	C3',C4'
1	1	4004	OMC	C4'
1	1	4009	2MA	C2',C3'
1	1	4010	PSU	C3',C4'
1	1	4058	OMU	C2',C3'
1	1	4086	PSU	C3',C4'
1	1	4111	PSU	C3',C4'

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	157	SER	Peptide
3	B	195	VAL	Peptide
10	I	116	MET	Peptide
12	K	93	GLN	Peptide
32	e	31	HIS	Peptide
38	k	102	MET	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	
3	B	269/271 (99%)	259 (96%)	10 (4%)	0	100	100
4	C	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
5	D	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
6	E	175/177 (99%)	159 (91%)	15 (9%)	1 (1%)	25	60
7	F	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
8	G	147/149 (99%)	134 (91%)	13 (9%)	0	100	100
9	H	128/130 (98%)	105 (82%)	23 (18%)	0	100	100
10	I	133/135 (98%)	120 (90%)	13 (10%)	0	100	100
11	J	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
12	K	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
13	L	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	M	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
15	N	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
16	O	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
17	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
18	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
19	R	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
20	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
21	T	92/94 (98%)	92 (100%)	0	0	100	100
22	U	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
23	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	W	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
25	X	75/77 (97%)	75 (100%)	0	0	100	100
26	Y	60/62 (97%)	60 (100%)	0	0	100	100
27	Z	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
28	a	64/66 (97%)	58 (91%)	6 (9%)	0	100	100
29	b	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
30	c	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
31	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
32	e	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	9	36
33	f	36/38 (95%)	36 (100%)	0	0	100	100
34	g	223/225 (99%)	212 (95%)	11 (5%)	0	100	100
35	h	206/208 (99%)	190 (92%)	16 (8%)	0	100	100
36	i	203/205 (99%)	200 (98%)	3 (2%)	0	100	100
37	j	154/156 (99%)	136 (88%)	18 (12%)	0	100	100
38	k	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
39	l	149/151 (99%)	144 (97%)	5 (3%)	0	100	100
40	m	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
41	n	125/127 (98%)	112 (90%)	13 (10%)	0	100	100
42	o	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
43	p	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
44	q	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
45	r	114/116 (98%)	103 (90%)	11 (10%)	0	100	100
46	s	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
47	t	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	13	43
48	u	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
49	v	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
50	w	64/66 (97%)	61 (95%)	3 (5%)	0	100	100
51	x	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
52	y	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
53	z	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
All	All	5869/5972 (98%)	5563 (95%)	303 (5%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	e	32	ILE
6	E	177	PHE
47	t	22	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	216/216 (100%)	213 (99%)	3 (1%)	67	86
4	C	164/164 (100%)	161 (98%)	3 (2%)	59	82
5	D	165/165 (100%)	162 (98%)	3 (2%)	59	82
6	E	148/148 (100%)	148 (100%)	0	100	100
7	F	136/136 (100%)	133 (98%)	3 (2%)	52	79
8	G	114/114 (100%)	111 (97%)	3 (3%)	46	75
9	H	99/99 (100%)	99 (100%)	0	100	100
10	I	104/104 (100%)	102 (98%)	2 (2%)	57	81
11	J	116/116 (100%)	116 (100%)	0	100	100
12	K	104/104 (100%)	103 (99%)	1 (1%)	76	90
13	L	103/103 (100%)	101 (98%)	2 (2%)	57	81
14	M	109/109 (100%)	109 (100%)	0	100	100
15	N	99/99 (100%)	99 (100%)	0	100	100
16	O	86/86 (100%)	84 (98%)	2 (2%)	50	78
17	P	99/99 (100%)	98 (99%)	1 (1%)	76	90
18	Q	89/89 (100%)	88 (99%)	1 (1%)	73	89
19	R	84/84 (100%)	82 (98%)	2 (2%)	49	77
20	S	93/93 (100%)	93 (100%)	0	100	100
21	T	81/81 (100%)	81 (100%)	0	100	100
22	U	84/84 (100%)	84 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	V	78/78 (100%)	77 (99%)	1 (1%)	69	87
24	W	58/58 (100%)	57 (98%)	1 (2%)	60	83
25	X	67/67 (100%)	66 (98%)	1 (2%)	65	85
26	Y	54/54 (100%)	54 (100%)	0	100	100
27	Z	48/48 (100%)	47 (98%)	1 (2%)	53	80
28	a	59/59 (100%)	57 (97%)	2 (3%)	37	69
29	b	47/47 (100%)	46 (98%)	1 (2%)	53	80
30	c	47/47 (100%)	46 (98%)	1 (2%)	53	80
31	d	38/38 (100%)	38 (100%)	0	100	100
32	e	51/51 (100%)	50 (98%)	1 (2%)	55	80
33	f	34/34 (100%)	34 (100%)	0	100	100
34	g	187/187 (100%)	187 (100%)	0	100	100
35	h	171/171 (100%)	168 (98%)	3 (2%)	59	82
36	i	172/172 (100%)	172 (100%)	0	100	100
37	j	119/119 (100%)	115 (97%)	4 (3%)	37	69
38	k	91/91 (100%)	90 (99%)	1 (1%)	73	89
39	l	124/124 (100%)	122 (98%)	2 (2%)	62	84
40	m	104/104 (100%)	103 (99%)	1 (1%)	76	90
41	n	105/105 (100%)	102 (97%)	3 (3%)	42	73
42	o	86/86 (100%)	85 (99%)	1 (1%)	71	88
43	p	90/90 (100%)	88 (98%)	2 (2%)	52	79
44	q	102/102 (100%)	101 (99%)	1 (1%)	76	90
45	r	94/94 (100%)	94 (100%)	0	100	100
46	s	83/83 (100%)	83 (100%)	0	100	100
47	t	76/76 (100%)	73 (96%)	3 (4%)	32	65
48	u	65/65 (100%)	64 (98%)	1 (2%)	65	85
49	v	74/74 (100%)	74 (100%)	0	100	100
50	w	57/57 (100%)	57 (100%)	0	100	100
51	x	72/72 (100%)	70 (97%)	2 (3%)	43	74
52	y	65/65 (100%)	64 (98%)	1 (2%)	65	85
53	z	60/60 (100%)	60 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4871/4871 (100%)	4811 (99%)	60 (1%)	72	88

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	80	ARG
3	B	204	VAL
3	B	260	ASN
4	C	33	ARG
4	C	136	ASN
4	C	151	THR
5	D	44	ARG
5	D	163	ASN
5	D	178	VAL
7	F	38	ASN
7	F	73	ASN
7	F	176	LYS
8	G	11	ASN
8	G	12	LEU
8	G	41	LYS
10	I	10	LEU
10	I	126	ARG
12	K	17	ARG
13	L	48	ARG
13	L	126	ARG
16	O	19	GLN
16	O	94	ARG
17	P	51	ARG
18	Q	92	ARG
19	R	10	LYS
19	R	48	LYS
23	V	24	ASN
24	W	14	ARG
25	X	27	ARG
27	Z	31	ARG
28	a	20	ASN
28	a	59	ARG
29	b	10	ARG
30	c	26	ASN
32	e	55	LEU
35	h	72	ARG
35	h	164	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	h	172	ARG
37	j	29	ARG
37	j	69	ARG
37	j	93	ARG
37	j	132	ASN
38	k	54	LEU
39	l	97	ASN
39	l	130	ASN
40	m	83	LEU
41	n	106	ARG
41	n	113	ARG
41	n	130	ARG
42	o	5	ARG
43	p	13	ARG
43	p	56	ARG
44	q	86	ARG
47	t	20	ASN
47	t	70	LEU
47	t	72	ARG
48	u	1	MET
51	x	32	ARG
51	x	78	ARG
52	y	54	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	134	ASN
3	B	251	GLN
3	B	260	ASN
4	C	32	ASN
4	C	136	ASN
4	C	150	GLN
5	D	163	ASN
7	F	88	GLN
8	G	43	ASN
10	I	110	GLN
15	N	31	HIS
16	O	38	GLN
19	R	86	GLN
20	S	61	ASN
21	T	48	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	V	24	ASN
26	Y	15	ASN
27	Z	20	HIS
28	a	20	ASN
30	c	26	ASN
34	g	39	HIS
37	j	132	ASN
38	k	63	ASN
39	l	97	ASN
39	l	130	ASN
40	m	4	GLN
40	m	18	GLN
44	q	5	ASN
46	s	43	ASN
47	t	20	ASN
47	t	40	GLN
51	x	57	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	4435/4458 (99%)	953 (21%)	24 (0%)
2	3	119/120 (99%)	25 (21%)	0
All	All	4554/4578 (99%)	978 (21%)	24 (0%)

All (978) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	7	A
1	1	9	G
1	1	19	A
1	1	22	G
1	1	32	A
1	1	33	A
1	1	39	G
1	1	47	C
1	1	48	C
1	1	51	A
1	1	54	C
1	1	56	U
1	1	68	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	70	U
1	1	71	A
1	1	73	C
1	1	74	A
1	1	81	A
1	1	83	C
1	1	84	U
1	1	85	U
1	1	86	G
1	1	87	C
1	1	88	U
1	1	89	U
1	1	94	G
1	1	95	C
1	1	96	U
1	1	97	G
1	1	98	A
1	1	115	G
1	1	116	A
1	1	120	A
1	1	121	U
1	1	122	G
1	1	129	A
1	1	131	A
1	1	135	C
1	1	141	G
1	1	144	G
1	1	149	A
1	1	151	A
1	1	160	A
1	1	163	C
1	1	177	G
1	1	181	A
1	1	182	A
1	1	183	C
1	1	195	A
1	1	197	A
1	1	204	G
1	1	207	C
1	1	211	G
1	1	212	G
1	1	226	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	232	G
1	1	245	U
1	1	247	G
1	1	251	G
1	1	266	G
1	1	267	C
1	1	279	A
1	1	280	C
1	1	289	G
1	1	298	A
1	1	299	G
1	1	321	A
1	1	328	C
1	1	332	G
1	1	345	C
1	1	347	G
1	1	352	C
1	1	354	G
1	1	362	G
1	1	367	U
1	1	372	C
1	1	384	G
1	1	392	C
1	1	406	G
1	1	408	A
1	1	411	A
1	1	412	A
1	1	413	G
1	1	421	U
1	1	422	C
1	1	424	G
1	1	429	U
1	1	435	A
1	1	447	G
1	1	448	A
1	1	451	A
1	1	455	G
1	1	456	A
1	1	457	G
1	1	458	U
1	1	463	U
1	1	464	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	465	A
1	1	467	U
1	1	468	A
1	1	469	C
1	1	474	G
1	1	475	C
1	1	476	U
1	1	478	A
1	1	481	G
1	1	482	A
1	1	484	G
1	1	486	U
1	1	496	A
1	1	498	A
1	1	499	A
1	1	505	G
1	1	509	A
1	1	510	A
1	1	511	C
1	1	513	C
1	1	516	PSU
1	1	517	G
1	1	518	C
1	1	519	C
1	1	527	7MG
1	1	528	C
1	1	531	U
1	1	532	A
1	1	533	A
1	1	539	A
1	1	547	A
1	1	559	A
1	1	562	U
1	1	568	G
1	1	570	G
1	1	572	A
1	1	573	A
1	1	576	C
1	1	577	G
1	1	579	A
1	1	607	A
1	1	625	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	628	G
1	1	633	G
1	1	650	G
1	1	653	U
1	1	654	G
1	1	656	G
1	1	660	C
1	1	665	A
1	1	686	U
1	1	700	G
1	1	702	A
1	1	703	G
1	1	718	A
1	1	721	G
1	1	723	U
1	1	724	G
1	1	731	G
1	1	734	G
1	1	735	C
1	1	747	A
1	1	749	A
1	1	755	G
1	1	758	C
1	1	760	G
1	1	777	A
1	1	781	A
1	1	793	U
1	1	794	A
1	1	814	A
1	1	815	A
1	1	817	C
1	1	821	G
1	1	827	U
1	1	828	U
1	1	839	C
1	1	841	C
1	1	842	U
1	1	843	U
1	1	844	G
1	1	846	G
1	1	849	G
1	1	857	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	864	A
1	1	876	C
1	1	883	C
1	1	887	G
1	1	914	A
1	1	926	G
1	1	934	C
1	1	942	G
1	1	960	U
1	1	961	U
1	1	963	G
1	1	966	2MG
1	1	969	A
1	1	971	G
1	1	975	A
1	1	976	G
1	1	977	A
1	1	982	U
1	1	989	U
1	1	992	U
1	1	993	G
1	1	996	A
1	1	1004	A
1	1	1005	A
1	1	1009	U
1	1	1017	U
1	1	1018	G
1	1	1025	U
1	1	1026	G
1	1	1028	C
1	1	1029	U
1	1	1030	U
1	1	1031	C
1	1	1032	G
1	1	1033	G
1	1	1035	A
1	1	1037	C
1	1	1040	U
1	1	1044	A
1	1	1045	C
1	1	1065	U
1	1	1071	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1081	A
1	1	1085	U
1	1	1094	G
1	1	1095	U
1	1	1101	A
1	1	1124	G
1	1	1125	U
1	1	1129	C
1	1	1132	C
1	1	1133	G
1	1	1136	C
1	1	1137	C
1	1	1138	G
1	1	1139	G
1	1	1140	C
1	1	1141	C
1	1	1142	G
1	1	1143	G
1	1	1145	A
1	1	1146	A
1	1	1154	G
1	1	1157	A
1	1	1158	C
1	1	1160	G
1	1	1161	C
1	1	1163	A
1	1	1171	A
1	1	1174	G
1	1	1175	G
1	1	1176	A
1	1	1188	A
1	1	1196	A
1	1	1197	A
1	1	1199	U
1	1	1202	U
1	1	1212	U
1	1	1213	A
1	1	1214	C
1	1	1226	C
1	1	1227	A
1	1	1228	C
1	1	1238	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1256	A
1	1	1257	A
1	1	1258	G
1	1	1265	C
1	1	1275	A
1	1	1279	G
1	1	1280	A
1	1	1286	U
1	1	1287	A
1	1	1298	U
1	1	1299	A
1	1	1302	C
1	1	1305	G
1	1	1308	U
1	1	1310	G
1	1	1311	A
1	1	1312	G
1	1	1315	U
1	1	1317	C
1	1	1318	A
1	1	1319	A
1	1	1320	C
1	1	1322	C
1	1	1335	U
1	1	1346	A
1	1	1357	A
1	1	1358	U
1	1	1363	A
1	1	1364	U
1	1	1370	G
1	1	1379	G
1	1	1381	U
1	1	1383	C
1	1	1394	A
1	1	1397	C
1	1	1398	A
1	1	1401	G
1	1	1403	C
1	1	1419	G
1	1	1429	A
1	1	1432	G
1	1	1440	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1441	A
1	1	1443	C
1	1	1446	A
1	1	1450	G
1	1	1451	G
1	1	1452	U
1	1	1453	C
1	1	1454	A
1	1	1455	A
1	1	1456	C
1	1	1457	A
1	1	1459	C
1	1	1460	C
1	1	1461	G
1	1	1462	U
1	1	1463	U
1	1	1464	U
1	1	1465	G
1	1	1471	A
1	1	1478	C
1	1	1481	A
1	1	1482	U
1	1	1483	G
1	1	1489	U
1	1	1490	G
1	1	1491	A
1	1	1501	U
1	1	1503	G
1	1	1504	A
1	1	1505	G
1	1	1506	A
1	1	1516	A
1	1	1521	G
1	1	1539	C
1	1	1540	U
1	1	1541	G
1	1	1552	G
1	1	1555	A
1	1	1558	A
1	1	1564	G
1	1	1567	C
1	1	1577	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1578	U
1	1	1580	A
1	1	1581	G
1	1	1586	G
1	1	1590	A
1	1	1591	G
1	1	1594	G
1	1	1607	A
1	1	1608	U
1	1	1609	A
1	1	1624	A
1	1	1625	A
1	1	1626	U
1	1	1631	A
1	1	1645	U
1	1	1646	C
1	1	1664	U
1	1	1669	C
1	1	1671	A
1	1	1676	U
1	1	1677	U
1	1	1687	A
1	1	1702	A
1	1	1705	A
1	1	1721	G
1	1	1722	A
1	1	1728	A
1	1	1730	U
1	1	1731	C
1	1	1732	A
1	1	1733	A
1	1	1754	G
1	1	1755	C
1	1	1756	G
1	1	1770	C
1	1	1771	A
1	1	1772	G
1	1	1781	C
1	1	1782	U
1	1	1783	G
1	1	1784	A
1	1	1788	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1791	G
1	1	1793	G
1	1	1810	U
1	1	1816	A
1	1	1817	A
1	1	1828	A
1	1	1831	G
1	1	1835	G
1	1	1836	A
1	1	1838	A
1	1	1840	C
1	1	1851	A
1	1	1862	G
1	1	1867	G
1	1	1868	A
1	1	1869	G
1	1	1877	A
1	1	1878	G
1	1	1881	G
1	1	1889	C
1	1	1892	G
1	1	1902	G
1	1	1905	U
1	1	1909	U
1	1	1910	A
1	1	1911	U
1	1	1917	G
1	1	1918	A
1	1	1930	G
1	1	1953	A
1	1	1954	U
1	1	1957	U
1	1	1963	A
1	1	1987	G
1	1	1996	C
1	1	1997	G
1	1	2002	G
1	1	2009	A
1	1	2011	A
1	1	2014	A
1	1	2015	C
1	1	2016	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2035	A
1	1	2036	G
1	1	2037	C
1	1	2038	A
1	1	2052	U
1	1	2053	A
1	1	2054	G
1	1	2055	G
1	1	2069	A
1	1	2079	U
1	1	2081	A
1	1	2086	U
1	1	2092	A
1	1	2108	A
1	1	2109	A
1	1	2115	A
1	1	2119	A
1	1	2120	A
1	1	2121	U
1	1	2122	A
1	1	2133	A
1	1	2142	G
1	1	2143	A
1	1	2151	C
1	1	2153	G
1	1	2159	U
1	1	2160	A
1	1	2161	A
1	1	2174	A
1	1	2176	A
1	1	2191	A
1	1	2192	U
1	1	2202	G
1	1	2216	U
1	1	2223	C
1	1	2232	G
1	1	2236	A
1	1	2244	G
1	1	2246	C
1	1	2251	1MG
1	1	2252	PSU
1	1	2253	5MU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2254	G
1	1	2270	A
1	1	2271	C
1	1	2281	G
1	1	2282	G
1	1	2285	U
1	1	2287	A
1	1	2288	A
1	1	2290	G
1	1	2291	G
1	1	2295	A
1	1	2297	C
1	1	2298	A
1	1	2299	A
1	1	2311	G
1	1	2312	C
1	1	2318	C
1	1	2325	A
1	1	2333	U
1	1	2334	U
1	1	2351	A
1	1	2352	U
1	1	2353	U
1	1	2364	G
1	1	2365	G
1	1	2383	A
1	1	2388	G
1	1	2389	G
1	1	2390	U
1	1	2391	C
1	1	2394	C
1	1	2398	A
1	1	2399	C
1	1	2401	U
1	1	2402	A
1	1	2416	A
1	1	2420	G
1	1	2433	A
1	1	2437	U
1	1	2447	A
1	1	2452	C
1	1	2461	PSU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2462	G
1	1	2467	C
1	1	2480	G
1	1	2489	A
1	1	2491	C
1	1	2495	G
1	1	2501	C
1	1	2502	A
1	1	2505	U
1	1	2515	A
1	1	2518	U
1	1	2519	C
1	1	2528	G
1	1	2532	G
1	1	2539	U
1	1	2546	A
1	1	2547	G
1	1	2548	G
1	1	2549	C
1	1	2550	C
1	1	2552	A
1	1	2553	G
1	1	2557	G
1	1	2560	A
1	1	2562	G
1	1	2563	A
1	1	2568	G
1	1	2569	G
1	1	2570	C
1	1	2572	U
1	1	2573	A
1	1	2574	G
1	1	2576	A
1	1	2577	G
1	1	2579	A
1	1	2584	U
1	1	2589	U
1	1	2590	A
1	1	2593	G
1	1	2594	A
1	1	2595	A
1	1	2601	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2602	A
1	1	2605	G
1	1	2607	U
1	1	2611	U
1	1	2613	G
1	1	2614	U
1	1	2617	A
1	1	2618	G
1	1	2622	G
1	1	2624	C
1	1	2625	U
1	1	2626	G
1	1	2628	G
1	1	2632	A
1	1	2636	U
1	1	2638	U
1	1	2639	A
1	1	2640	A
1	1	2641	C
1	1	2642	G
1	1	2648	A
1	1	2662	A
1	1	2663	G
1	1	2675	A
1	1	2676	C
1	1	2677	G
1	1	2678	C
1	1	2679	U
1	1	2681	A
1	1	2683	G
1	1	2684	C
1	1	2692	G
1	1	2710	A
1	1	2718	G
1	1	2742	G
1	1	2744	G
1	1	2746	U
1	1	2756	G
1	1	2759	A
1	1	2762	G
1	1	2763	C
1	1	2772	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2774	A
1	1	2777	G
1	1	2778	A
1	1	2779	U
1	1	2781	A
1	1	2790	A
1	1	2792	A
1	1	2795	C
1	1	2806	G
1	1	2807	A
1	1	2819	U
1	1	2821	C
1	1	2827	A
1	1	2835	U
1	1	2850	U
1	1	2851	C
1	1	2858	U
1	1	2871	A
1	1	2874	G
1	1	2880	G
1	1	2885	U
1	1	2886	G
1	1	2889	A
1	1	2901	A
1	1	2903	U
1	1	2904	C
1	1	2905	C
1	1	2917	U
1	1	2922	G
1	1	2923	C
1	1	2925	A
1	1	2934	C
1	1	2958	G
1	1	2959	A
1	1	2967	C
1	1	2984	G
1	1	2988	G
1	1	2995	C
1	1	2996	A
1	1	2999	C
1	1	3003	U
1	1	3004	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	3009	A
1	1	3013	C
1	1	3014	A
1	1	3015	A
1	1	3016	G
1	1	3021	A
1	1	3027	G
1	1	3028	A
1	1	3030	G
1	1	3041	A
1	1	3042	C
1	1	3043	G
1	1	3046	G
1	1	3066	G
1	1	3072	A
1	1	3075	A
1	1	3084	U
1	1	3089	A
1	1	3090	U
1	1	3091	C
1	1	3092	A
1	1	3095	U
1	1	3096	A
1	1	3113	C
1	1	3114	A
1	1	3116	A
1	1	3125	G
1	1	3136	A
1	1	3140	A
1	1	3153	U
1	1	3154	U
1	1	3155	G
1	1	3157	G
1	1	3173	G
1	1	3175	A
1	1	3180	G
1	1	3221	G
1	1	3234	C
1	1	3235	U
1	1	3236	C
1	1	3238	C
1	1	3239	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	3244	G
1	1	3263	A
1	1	3270	C
1	1	3279	A
1	1	3306	C
1	1	3307	A
1	1	3308	A
1	1	3314	A
1	1	3317	G
1	1	3322	C
1	1	3323	G
1	1	3335	A
1	1	3339	C
1	1	3353	A
1	1	3354	A
1	1	3370	U
1	1	3371	U
1	1	3376	C
1	1	3377	A
1	1	3378	A
1	1	3379	G
1	1	3406	A
1	1	3412	G
1	1	3413	G
1	1	3416	G
1	1	3417	PSU
1	1	3418	A
1	1	3419	A
1	1	3420	C
1	1	3423	PSU
1	1	3424	A
1	1	3429	U
1	1	3430	C
1	1	3435	G
1	1	3436	G
1	1	3442	A
1	1	3443	A
1	1	3444	A
1	1	3445	5MU
1	1	3446	U
1	1	3461	U
1	1	3472	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	3473	C
1	1	3476	A
1	1	3477	U
1	1	3478	G
1	1	3486	G
1	1	3497	U
1	1	3498	G
1	1	3499	U
1	1	3503	C
1	1	3508	G
1	1	3527	C
1	1	3528	U
1	1	3529	C
1	1	3533	G
1	1	3537	A
1	1	3538	G
1	1	3539	A
1	1	3541	G
1	1	3542	C
1	1	3549	C
1	1	3561	C
1	1	3562	G
1	1	3566	A
1	1	3567	G
1	1	3568	A
1	1	3575	G7M
1	1	3578	C
1	1	3599	G
1	1	3605	U
1	1	3606	G
1	1	3608	G
1	1	3611	U
1	1	3613	G
1	1	3614	A
1	1	3616	G
1	1	3617	U
1	1	3619	U
1	1	3621	G
1	1	3623	A
1	1	3624	U
1	1	3626	G
1	1	3629	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	3631	G
1	1	3632	A
1	1	3633	G
1	1	3637	U
1	1	3638	U
1	1	3639	G
1	1	3640	A
1	1	3642	G
1	1	3645	U
1	1	3649	C
1	1	3652	C
1	1	3653	A
1	1	3654	G
1	1	3655	U
1	1	3659	C
1	1	3661	U
1	1	3663	G
1	1	3664	A
1	1	3666	C
1	1	3668	G
1	1	3669	A
1	1	3670	C
1	1	3671	C
1	1	3676	A
1	1	3677	A
1	1	3678	U
1	1	3681	C
1	1	3685	C
1	1	3686	U
1	1	3688	U
1	1	3689	A
1	1	3693	U
1	1	3694	U
1	1	3695	U
1	1	3696	G
1	1	3700	U
1	1	3704	A
1	1	3710	G
1	1	3716	U
1	1	3717	A
1	1	3726	U
1	1	3731	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	3732	C
1	1	3744	G
1	1	3749	U
1	1	3756	G
1	1	3774	A
1	1	3779	A
1	1	3784	A
1	1	3789	C
1	1	3792	G
1	1	3793	A
1	1	3803	A
1	1	3811	U
1	1	3813	G
1	1	3815	A
1	1	3825	G
1	1	3828	A
1	1	3831	G
1	1	3833	A
1	1	3839	A
1	1	3840	U
1	1	3851	G
1	1	3853	C
1	1	3856	C
1	1	3858	A
1	1	3867	G
1	1	3889	G
1	1	3891	C
1	1	3897	G
1	1	3902	G
1	1	3908	U
1	1	3909	C
1	1	3910	U
1	1	3912	A
1	1	3929	U
1	1	3931	A
1	1	3932	A
1	1	3935	G
1	1	3936	A
1	1	3937	U
1	1	3941	A
1	1	3946	C
1	1	3947	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	3954	A
1	1	3963	PSU
1	1	3964	G
1	1	3976	G
1	1	3982	A
1	1	3984	A
1	1	3996	G
1	1	3997	U
1	1	4003	A
1	1	4004	OMC
1	1	4005	C
1	1	4008	G
1	1	4010	PSU
1	1	4011	G
1	1	4012	U
1	1	4018	C
1	1	4024	A
1	1	4026	C
1	1	4031	G
1	1	4035	G
1	1	4053	A
1	1	4058	OMU
1	1	4059	G
1	1	4060	U
1	1	4062	C
1	1	4072	A
1	1	4073	G
1	1	4075	G
1	1	4078	A
1	1	4079	C
1	1	4080	G
1	1	4086	PSU
1	1	4087	G
1	1	4088	G
1	1	4091	U
1	1	4108	A
1	1	4111	PSU
1	1	4112	C
1	1	4115	U
1	1	4119	U
1	1	4121	U
1	1	4135	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	4136	G
1	1	4152	C
1	1	4169	G
1	1	4193	U
1	1	4195	U
1	1	4196	U
1	1	4220	G
1	1	4222	C
1	1	4231	A
1	1	4232	A
1	1	4233	A
1	1	4238	G
1	1	4239	A
1	1	4245	U
1	1	4250	G
1	1	4254	A
1	1	4271	A
1	1	4283	G
1	1	4284	A
1	1	4299	C
1	1	4300	C
1	1	4304	U
1	1	4309	G
1	1	4324	U
1	1	4326	A
1	1	4327	A
1	1	4331	G
1	1	4341	A
1	1	4342	U
1	1	4355	U
1	1	4356	A
1	1	4357	A
1	1	4358	A
1	1	4359	C
1	1	4360	G
1	1	4361	G
1	1	4362	A
1	1	4364	A
1	1	4365	U
1	1	4366	G
1	1	4367	G
1	1	4368	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	4369	U
1	1	4370	G
1	1	4388	U
1	1	4391	G
1	1	4400	C
1	1	4408	A
1	1	4409	A
1	1	4410	G
1	1	4413	G
1	1	4415	A
1	1	4419	A
1	1	4422	U
1	1	4433	G
1	1	4445	G
1	1	4446	G
1	1	4450	A
2	3	2	G
2	3	5	U
2	3	9	G
2	3	13	G
2	3	16	G
2	3	24	G
2	3	25	U
2	3	35	C
2	3	36	C
2	3	42	C
2	3	44	G
2	3	45	A
2	3	51	G
2	3	56	G
2	3	57	A
2	3	65	U
2	3	66	A
2	3	68	C
2	3	88	C
2	3	89	U
2	3	90	C
2	3	99	A
2	3	105	G
2	3	109	A
2	3	120	U

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	496	A
1	1	516	PSU
1	1	527	7MG
1	1	1145	A
1	1	1461	G
1	1	1910	A
1	1	2192	U
1	1	2253	5MU
1	1	2290	G
1	1	2400	U
1	1	2461	PSU
1	1	2885	U
1	1	3417	PSU
1	1	3423	PSU
1	1	3445	5MU
1	1	3652	C
1	1	3668	G
1	1	3814	G
1	1	3931	A
1	1	3963	PSU
1	1	4004	OMC
1	1	4010	PSU
1	1	4086	PSU
1	1	4111	PSU

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	3TD	1	3421	1	18,22,23	2.84	8 (44%)	22,32,35	1.72	2 (9%)
1	2MG	1	966	1	18,26,27	2.88	5 (27%)	16,38,41	1.39	3 (18%)
1	UR3	1	4414	1	19,22,23	2.82	6 (31%)	26,32,35	1.45	3 (11%)
1	PSU	1	516	1	18,21,22	2.10	6 (33%)	22,30,33	2.20	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1	3963	1	18,21,22	2.29	5 (27%)	22,30,33	2.29	5 (22%)
1	1MG	1	2251	1	18,26,27	2.96	6 (33%)	19,39,42	2.37	9 (47%)
1	PSU	1	4086	1	18,21,22	2.17	5 (27%)	22,30,33	2.14	7 (31%)
1	5MU	1	2253	1	19,22,23	2.32	7 (36%)	28,32,35	4.01	13 (46%)
1	OMG	1	3757	1	18,26,27	2.91	8 (44%)	19,38,41	1.76	4 (21%)
1	5MC	1	967	1,54	18,22,23	2.01	3 (16%)	26,32,35	1.44	4 (15%)
1	7MG	1	527	1	22,26,27	6.31	6 (27%)	29,39,42	2.43	10 (34%)
1	PSU	1	2461	1	18,21,22	2.25	5 (27%)	22,30,33	2.22	5 (22%)
1	PSU	1	3423	1	18,21,22	2.11	5 (27%)	22,30,33	2.07	5 (22%)
1	5MC	1	3468	1	18,22,23	2.14	3 (16%)	26,32,35	1.41	4 (15%)
1	PSU	1	4111	1	18,21,22	2.18	5 (27%)	22,30,33	2.09	4 (18%)
1	6MZ	1	3124	1	18,25,26	1.98	1 (5%)	16,36,39	2.36	4 (25%)
1	OMU	1	4058	1	19,22,23	2.76	7 (36%)	26,31,34	2.38	12 (46%)
1	5MU	1	3445	1	19,22,23	2.52	7 (36%)	28,32,35	3.54	9 (32%)
1	2MG	1	1207	1	18,26,27	2.83	5 (27%)	16,38,41	1.44	3 (18%)
1	2MG	1	4432	1	18,26,27	2.89	6 (33%)	16,38,41	1.52	3 (18%)
1	G7M	1	3575	1	20,26,27	2.81	5 (25%)	17,39,42	1.23	2 (11%)
1	5MC	1	1407	1	18,22,23	2.05	3 (16%)	26,32,35	1.38	3 (11%)
1	MA6	1	4435	1	19,26,27	0.90	0	18,38,41	1.71	2 (11%)
1	2MG	1	3951	1	18,26,27	2.97	6 (33%)	16,38,41	1.36	3 (18%)
1	PSU	1	3417	1	18,21,22	1.97	5 (27%)	22,30,33	2.12	4 (18%)
1	2MA	1	4009	1,54	17,25,26	1.56	3 (17%)	17,37,40	1.44	2 (11%)
1	MA6	1	4434	1	19,26,27	0.97	1 (5%)	18,38,41	1.64	3 (16%)
1	6MZ	1	3536	1	18,25,26	2.12	1 (5%)	16,36,39	3.75	8 (50%)
1	OMC	1	4004	1,54	19,22,23	1.77	6 (31%)	26,31,34	2.10	9 (34%)
1	PSU	1	4010	1	18,21,22	2.35	5 (27%)	22,30,33	2.37	5 (22%)
1	4OC	1	1402	1	20,23,24	2.44	5 (25%)	26,32,35	2.32	9 (34%)
1	PSU	1	2252	1,54	18,21,22	2.25	6 (33%)	22,30,33	2.30	5 (22%)
44	0TD	q	89	44	7,9,10	1.40	0	6,11,13	2.82	3 (50%)
1	2MG	1	3341	1	18,26,27	2.85	6 (33%)	16,38,41	1.42	4 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	3TD	1	3421	1	1/1/5/5	4/7/25/26	0/2/2/2
1	2MG	1	966	1	-	4/5/27/28	0/3/3/3
1	UR3	1	4414	1	-	0/7/25/26	0/2/2/2
1	PSU	1	516	1	2/2/5/5	5/7/25/26	0/2/2/2
1	PSU	1	3963	1	2/2/5/5	3/7/25/26	0/2/2/2
1	1MG	1	2251	1	2/2/5/5	1/3/25/26	0/3/3/3
1	PSU	1	4086	1	2/2/5/5	3/7/25/26	0/2/2/2
1	5MU	1	2253	1	2/2/5/5	5/7/25/26	0/2/2/2
1	OMG	1	3757	1	1/1/5/5	2/5/27/28	0/3/3/3
1	5MC	1	967	1,54	-	0/7/25/26	0/2/2/2
1	7MG	1	527	1	1/1/7/7	3/7/37/38	0/3/3/3
1	PSU	1	2461	1	2/2/5/5	3/7/25/26	0/2/2/2
1	PSU	1	3423	1	2/2/5/5	3/7/25/26	0/2/2/2
1	5MC	1	3468	1	-	0/7/25/26	0/2/2/2
1	PSU	1	4111	1	2/2/5/5	3/7/25/26	0/2/2/2
1	6MZ	1	3124	1	2/2/5/6	5/5/27/28	0/3/3/3
1	OMU	1	4058	1	2/2/5/5	3/9/27/28	0/2/2/2
1	5MU	1	3445	1	2/2/5/5	1/7/25/26	0/2/2/2
1	2MG	1	1207	1	-	0/5/27/28	0/3/3/3
1	2MG	1	4432	1	-	0/5/27/28	0/3/3/3
1	G7M	1	3575	1	1/1/5/5	2/3/25/26	0/3/3/3
1	5MC	1	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	1	4435	1	-	3/7/29/30	0/3/3/3
1	2MG	1	3951	1	-	0/5/27/28	0/3/3/3
1	PSU	1	3417	1	2/2/5/5	3/7/25/26	0/2/2/2
1	2MA	1	4009	1,54	2/2/5/5	2/3/25/26	0/3/3/3
1	MA6	1	4434	1	-	1/7/29/30	0/3/3/3
1	6MZ	1	3536	1	2/2/5/6	2/5/27/28	0/3/3/3
1	OMC	1	4004	1,54	1/1/5/5	4/9/27/28	0/2/2/2
1	PSU	1	4010	1	2/2/5/5	3/7/25/26	0/2/2/2
1	4OC	1	1402	1	2/2/5/6	4/9/29/30	0/2/2/2
1	PSU	1	2252	1,54	2/2/5/5	3/7/25/26	0/2/2/2
44	0TD	q	89	44	-	1/7/12/14	-
1	2MG	1	3341	1	-	0/5/27/28	0/3/3/3

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	527	7MG	C8-N9	-27.11	1.30	1.46
1	1	3575	G7M	O6-C6	9.70	1.43	1.23
1	1	966	2MG	O6-C6	8.88	1.41	1.23
1	1	3757	OMG	O6-C6	8.71	1.41	1.23
1	1	1207	2MG	O6-C6	8.70	1.41	1.23
1	1	1402	4OC	O2-C2	8.64	1.39	1.23
1	1	4432	2MG	O6-C6	8.44	1.40	1.23
1	1	4414	UR3	O4-C4	8.37	1.41	1.23
1	1	2251	1MG	O6-C6	8.34	1.38	1.22
1	1	3951	2MG	O6-C6	8.29	1.40	1.23
1	1	3341	2MG	O6-C6	8.28	1.40	1.23
1	1	3421	3TD	O4-C4	8.00	1.40	1.23
1	1	527	7MG	O6-C6	7.78	1.38	1.23
1	1	4058	OMU	O4-C4	7.62	1.39	1.24
1	1	3124	6MZ	C6-N6	7.33	1.47	1.35
1	1	3536	6MZ	C6-N6	7.20	1.46	1.35
1	1	527	7MG	C2-N2	6.38	1.49	1.34
1	1	967	5MC	C4-N4	6.36	1.50	1.34
1	1	3468	5MC	C4-N4	6.31	1.50	1.34
1	1	1407	5MC	C4-N4	6.18	1.50	1.34
1	1	3445	5MU	C2-N1	-6.05	1.28	1.38
1	1	966	2MG	C2-N2	5.95	1.46	1.33
1	1	4432	2MG	C2-N2	5.66	1.46	1.33
1	1	1207	2MG	C2-N2	5.65	1.46	1.33
1	1	3951	2MG	C2-N2	5.63	1.45	1.33
1	1	2251	1MG	C2-N2	5.49	1.44	1.34
1	1	3341	2MG	C2-N2	5.26	1.45	1.33
1	1	3468	5MC	C2-N1	-5.11	1.28	1.40
1	1	4010	PSU	C4-N3	-5.09	1.29	1.38
1	1	516	PSU	C4-N3	-5.09	1.29	1.38
1	1	3963	PSU	C4-N3	-5.08	1.29	1.38
1	1	4086	PSU	C4-N3	-5.05	1.29	1.38
1	1	2252	PSU	C4-N3	-5.04	1.29	1.38
1	1	2461	PSU	C4-N3	-5.01	1.29	1.38
1	1	3423	PSU	C4-N3	-4.94	1.29	1.38
1	1	4111	PSU	C4-N3	-4.91	1.29	1.38
1	1	2251	1MG	C6-N1	-4.89	1.30	1.39
1	1	3963	PSU	C2-N1	-4.84	1.30	1.36
1	1	3575	G7M	C6-N1	-4.82	1.30	1.37
1	1	3421	3TD	C2-N1	-4.69	1.31	1.37
1	1	2253	5MU	C2-N1	-4.65	1.31	1.38
1	1	4010	PSU	C2-N1	-4.64	1.30	1.36
1	1	1407	5MC	C2-N1	-4.61	1.30	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	3575	G7M	C2-N2	4.57	1.45	1.34
1	1	3445	5MU	C2-N3	-4.54	1.29	1.38
1	1	3417	PSU	C4-N3	-4.53	1.30	1.38
1	1	4010	PSU	C6-C5	4.47	1.40	1.35
1	1	3757	OMG	C6-N1	-4.46	1.31	1.37
1	1	3951	2MG	C6-N1	-4.44	1.31	1.37
1	1	967	5MC	C2-N1	-4.43	1.30	1.40
1	1	3757	OMG	C2-N2	4.37	1.44	1.34
1	1	2252	PSU	C6-C5	4.35	1.40	1.35
1	1	2461	PSU	C2-N1	-4.30	1.30	1.36
1	1	4086	PSU	C2-N1	-4.28	1.30	1.36
1	1	4058	OMU	C2-N3	-4.27	1.30	1.38
1	1	4432	2MG	C6-N1	-4.26	1.31	1.37
1	1	4414	UR3	C4-N3	-4.26	1.31	1.40
1	1	4414	UR3	C2-N1	-4.26	1.32	1.38
1	1	4111	PSU	C2-N1	-4.25	1.31	1.36
1	1	3341	2MG	C6-N1	-4.22	1.31	1.37
1	1	4058	OMU	C4-N3	-4.22	1.31	1.38
1	1	2253	5MU	C2-N3	-4.21	1.30	1.38
1	1	3963	PSU	C6-N1	-4.19	1.29	1.36
1	1	2252	PSU	C2-N1	-4.15	1.31	1.36
1	1	4004	OMC	C4-N4	4.13	1.43	1.33
1	1	1402	4OC	C4-N4	4.11	1.44	1.35
1	1	4058	OMU	C2-N1	-4.07	1.31	1.38
1	1	516	PSU	C6-C5	4.04	1.40	1.35
1	1	3423	PSU	C6-C5	4.02	1.40	1.35
1	1	4009	2MA	C6-N6	4.02	1.45	1.28
1	1	527	7MG	C4-N9	-4.01	1.33	1.37
1	1	2461	PSU	C6-C5	3.99	1.40	1.35
1	1	3421	3TD	C4-N3	-3.92	1.32	1.40
1	1	4010	PSU	C6-N1	-3.92	1.29	1.36
1	1	4086	PSU	C6-N1	-3.91	1.29	1.36
1	1	3423	PSU	C2-N1	-3.83	1.31	1.36
1	1	4111	PSU	C6-N1	-3.81	1.29	1.36
1	1	2461	PSU	C6-N1	-3.81	1.29	1.36
1	1	3951	2MG	C5-C6	-3.75	1.39	1.47
1	1	4111	PSU	C6-C5	3.68	1.39	1.35
1	1	3417	PSU	C2-N1	-3.65	1.31	1.36
1	1	2253	5MU	O2-C2	-3.64	1.16	1.23
1	1	3963	PSU	C6-C5	3.61	1.39	1.35
1	1	3417	PSU	C6-C5	3.61	1.39	1.35
1	1	3417	PSU	C6-N1	-3.54	1.30	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	4414	UR3	C2-N3	-3.53	1.32	1.39
1	1	3445	5MU	C6-C5	3.53	1.40	1.34
1	1	4058	OMU	O2-C2	-3.52	1.16	1.23
1	1	2252	PSU	C6-N1	-3.51	1.30	1.36
1	1	4414	UR3	O2-C2	-3.49	1.16	1.22
1	1	3445	5MU	C6-N1	-3.46	1.32	1.38
1	1	1207	2MG	C6-N1	-3.46	1.32	1.37
1	1	3423	PSU	C6-N1	-3.43	1.30	1.36
1	1	3341	2MG	C2-N1	-3.41	1.31	1.36
1	1	2253	5MU	C6-C5	3.37	1.40	1.34
1	1	3445	5MU	O2-C2	-3.33	1.17	1.23
1	1	966	2MG	C6-N1	-3.30	1.32	1.37
1	1	3445	5MU	O4-C4	-3.30	1.17	1.23
1	1	2253	5MU	C4-N3	-3.30	1.32	1.38
1	1	4086	PSU	C6-C5	3.29	1.39	1.35
1	1	4004	OMC	C5-C4	-3.28	1.35	1.42
1	1	3445	5MU	C4-N3	-3.27	1.32	1.38
1	1	3951	2MG	C2-N1	-3.22	1.31	1.36
1	1	2253	5MU	C6-N1	-3.22	1.32	1.38
1	1	516	PSU	C6-N1	-3.20	1.30	1.36
1	1	527	7MG	C6-N1	-3.19	1.32	1.38
1	1	516	PSU	C2-N1	-3.11	1.32	1.36
1	1	2253	5MU	O4-C4	-3.10	1.17	1.23
1	1	3341	2MG	C5-C6	-3.03	1.41	1.47
1	1	2461	PSU	C2-N3	-3.02	1.32	1.37
1	1	3421	3TD	C2-N3	-3.01	1.31	1.38
1	1	3421	3TD	C6-C5	2.98	1.38	1.35
1	1	516	PSU	C2-N3	-2.98	1.32	1.37
1	1	966	2MG	C5-C6	-2.93	1.41	1.47
1	1	1402	4OC	C2-N1	-2.91	1.33	1.40
1	1	2252	PSU	C2-N3	-2.90	1.32	1.37
1	1	4086	PSU	C2-N3	-2.90	1.32	1.37
1	1	2251	1MG	C5-C6	-2.90	1.38	1.47
1	1	1207	2MG	C5-C6	-2.90	1.41	1.47
1	1	4004	OMC	O2-C2	-2.89	1.18	1.23
1	1	4432	2MG	C5-C6	-2.89	1.41	1.47
1	1	4432	2MG	C2-N1	-2.88	1.32	1.36
1	1	3421	3TD	O2-C2	-2.86	1.17	1.23
1	1	3757	OMG	C2-N1	-2.85	1.30	1.37
1	1	4111	PSU	C2-N3	-2.83	1.32	1.37
1	1	4010	PSU	C2-N3	-2.78	1.32	1.37
1	1	3757	OMG	C5-C6	-2.76	1.41	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	4414	UR3	C6-N1	-2.76	1.31	1.38
1	1	527	7MG	C2-N1	-2.75	1.30	1.37
1	1	1207	2MG	C2-N1	-2.75	1.32	1.36
1	1	2251	1MG	C8-N7	-2.74	1.30	1.35
1	1	4058	OMU	C5-C4	-2.70	1.37	1.43
1	1	1407	5MC	C2-N3	-2.65	1.31	1.36
1	1	4009	2MA	C5-C4	-2.64	1.36	1.43
1	1	4004	OMC	C2-N1	-2.60	1.34	1.40
1	1	3757	OMG	O2'-CM2	-2.59	1.33	1.42
1	1	3951	2MG	C5-C4	-2.55	1.36	1.43
1	1	3421	3TD	C6-N1	-2.54	1.32	1.36
1	1	3423	PSU	C2-N3	-2.50	1.33	1.37
1	1	3963	PSU	C2-N3	-2.49	1.33	1.37
1	1	3468	5MC	C2-N3	-2.47	1.31	1.36
1	1	3421	3TD	O4'-C1'	-2.44	1.40	1.43
1	1	3575	G7M	C2-N1	-2.43	1.31	1.37
1	1	4009	2MA	C6-N1	-2.38	1.32	1.38
1	1	4058	OMU	C6-N1	-2.38	1.32	1.38
1	1	966	2MG	C2-N1	-2.38	1.32	1.36
1	1	3757	OMG	C5-C4	-2.37	1.37	1.43
1	1	1402	4OC	C2-N3	-2.37	1.31	1.36
1	1	2251	1MG	C5-C4	-2.35	1.37	1.43
1	1	3417	PSU	C2-N3	-2.34	1.33	1.37
1	1	4004	OMC	C2-N3	-2.27	1.31	1.36
1	1	1402	4OC	C6-N1	-2.26	1.32	1.38
1	1	4432	2MG	C5-C4	-2.26	1.37	1.43
1	1	967	5MC	C2-N3	-2.25	1.31	1.36
1	1	516	PSU	O4'-C1'	-2.20	1.40	1.43
1	1	3341	2MG	C5-C4	-2.15	1.37	1.43
1	1	3757	OMG	C8-N7	-2.09	1.31	1.35
1	1	4434	MA6	C8-N7	-2.08	1.31	1.34
1	1	3575	G7M	C8-N7	-2.08	1.29	1.33
1	1	2252	PSU	O4'-C1'	-2.05	1.41	1.43
1	1	4004	OMC	C4-N3	-2.05	1.30	1.34

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2253	5MU	N3-C2-N1	9.66	127.72	114.89
1	1	2253	5MU	C5M-C5-C4	9.47	129.19	118.77
1	1	3445	5MU	C5M-C5-C4	8.86	128.52	118.77
1	1	3536	6MZ	C9-N6-C6	-8.64	115.43	122.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3445	5MU	N3-C2-N1	8.41	126.06	114.89
1	1	3445	5MU	C4-N3-C2	-7.58	117.54	127.35
1	1	2253	5MU	C5M-C5-C6	-7.31	113.09	122.85
1	1	2253	5MU	C4-N3-C2	-7.26	117.95	127.35
1	1	2252	PSU	N1-C2-N3	6.78	122.81	115.13
1	1	3536	6MZ	C2-N1-C6	6.61	122.26	116.59
1	1	3124	6MZ	C2-N1-C6	6.56	122.22	116.59
1	1	3445	5MU	C5M-C5-C6	-6.35	114.37	122.85
1	1	4010	PSU	C6-C5-C4	-6.34	113.77	118.20
1	1	516	PSU	N1-C2-N3	6.31	122.28	115.13
1	1	3963	PSU	N1-C2-N3	6.28	122.24	115.13
1	1	2253	5MU	C1'-N1-C2	6.22	128.82	117.57
1	1	3423	PSU	N1-C2-N3	6.20	122.15	115.13
1	1	3421	3TD	N1-C2-N3	6.17	121.01	116.14
1	1	527	7MG	N9-C4-N3	6.06	134.53	125.47
1	1	2461	PSU	N1-C2-N3	5.96	121.89	115.13
1	1	4086	PSU	N1-C2-N3	5.93	121.85	115.13
1	1	4004	OMC	O2-C2-N3	-5.91	112.71	122.33
1	1	3445	5MU	C5-C4-N3	5.88	120.33	115.31
1	1	3417	PSU	N1-C2-N3	5.78	121.68	115.13
1	1	4010	PSU	N1-C2-N3	5.55	121.42	115.13
1	1	4111	PSU	N1-C2-N3	5.39	121.24	115.13
44	q	89	0TD	OD2-CG-CB	5.38	124.77	113.15
1	1	4435	MA6	N3-C2-N1	-5.32	120.37	128.68
1	1	4414	UR3	C4-N3-C2	-5.30	119.57	124.56
1	1	1402	4OC	C1'-N1-C2	5.30	130.24	118.42
1	1	2253	5MU	O2-C2-N3	-5.25	111.72	121.50
1	1	527	7MG	C5-C6-N1	5.25	120.24	110.99
1	1	3445	5MU	C5-C6-N1	-5.19	117.99	123.34
1	1	3963	PSU	O2-C2-N1	-5.16	117.11	122.79
1	1	3536	6MZ	N3-C2-N1	-5.12	120.67	128.68
1	1	1402	4OC	O2-C2-N3	-5.12	113.99	122.33
1	1	3124	6MZ	N3-C2-N1	-5.05	120.79	128.68
1	1	3536	6MZ	O3'-C3'-C4'	4.94	125.33	111.05
1	1	4434	MA6	N3-C2-N1	-4.89	121.03	128.68
1	1	4058	OMU	N3-C2-N1	4.89	121.38	114.89
1	1	3468	5MC	C5-C6-N1	-4.84	118.35	123.34
1	1	527	7MG	C2-N3-C4	4.83	120.90	112.30
1	1	2461	PSU	C6-C5-C4	-4.75	114.88	118.20
1	1	1402	4OC	C1'-N1-C6	-4.69	110.62	120.84
1	1	2253	5MU	C1'-N1-C6	-4.58	113.50	121.12
1	1	4111	PSU	C6-C5-C4	-4.49	115.06	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	527	7MG	C5-C4-N3	-4.46	119.62	128.13
1	1	2253	5MU	C5-C4-N3	4.38	119.05	115.31
1	1	3417	PSU	O2-C2-N1	-4.35	118.00	122.79
1	1	516	PSU	C4-N3-C2	-4.32	120.12	126.34
1	1	4058	OMU	C4-N3-C2	-4.29	120.92	126.58
1	1	4010	PSU	O2-C2-N1	-4.28	118.07	122.79
1	1	967	5MC	C5-C6-N1	-4.26	118.95	123.34
1	1	2251	1MG	O3'-C3'-C4'	4.23	123.29	111.05
1	1	4058	OMU	C1'-N1-C2	4.20	125.18	117.57
1	1	4058	OMU	O3'-C3'-C4'	4.20	123.18	111.05
1	1	3417	PSU	C4-N3-C2	-4.17	120.33	126.34
1	1	2251	1MG	O2'-C2'-C3'	4.17	125.30	111.82
1	1	2253	5MU	C6-N1-C2	-4.09	117.16	121.30
1	1	2252	PSU	C4-N3-C2	-4.00	120.58	126.34
1	1	3536	6MZ	C1'-N9-C4	-3.98	119.65	126.64
1	1	1407	5MC	O2-C2-N3	-3.90	115.99	122.33
1	1	3757	OMG	CM2-O2'-C2'	-3.85	104.42	114.52
1	1	2252	PSU	O2-C2-N1	-3.81	118.59	122.79
1	1	527	7MG	N9-C8-N7	3.79	108.81	103.38
1	1	3423	PSU	O2-C2-N1	-3.78	118.63	122.79
1	1	4058	OMU	C5-C4-N3	3.78	120.49	114.84
1	1	3963	PSU	C4-N3-C2	-3.77	120.91	126.34
1	1	4086	PSU	C4-N3-C2	-3.72	120.98	126.34
1	1	4004	OMC	C6-N1-C2	-3.70	114.07	120.49
1	1	4434	MA6	C4-C5-N7	-3.66	105.58	109.40
1	1	4432	2MG	C5-C6-N1	3.66	120.41	113.95
1	1	4004	OMC	O2-C2-N1	3.66	126.44	118.89
1	1	3445	5MU	O2-C2-N3	-3.61	114.78	121.50
1	1	1402	4OC	C2'-C1'-N1	3.59	121.19	114.22
1	1	4111	PSU	C4-N3-C2	-3.58	121.18	126.34
1	1	967	5MC	O2-C2-N3	-3.58	116.51	122.33
1	1	3536	6MZ	C4-C5-N7	-3.58	105.67	109.40
1	1	3445	5MU	O4-C4-N3	-3.57	113.28	120.12
1	1	516	PSU	C6-C5-C4	-3.56	115.71	118.20
1	1	3341	2MG	C5-C6-N1	3.55	120.22	113.95
1	1	4009	2MA	C5-C6-N1	3.54	120.14	114.02
1	1	4435	MA6	C4-C5-N7	-3.54	105.71	109.40
1	1	2461	PSU	O2-C2-N1	-3.50	118.93	122.79
1	1	4086	PSU	O2-C2-N1	-3.48	118.96	122.79
1	1	4111	PSU	O2-C2-N1	-3.48	118.96	122.79
1	1	3951	2MG	C5-C6-N1	3.48	120.09	113.95
1	1	1407	5MC	C5-C6-N1	-3.47	119.77	123.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3757	OMG	C5-C6-N1	3.42	119.98	113.95
1	1	3536	6MZ	C3'-C2'-C1'	-3.41	95.84	100.98
1	1	1207	2MG	C5-C6-N1	3.41	119.97	113.95
1	1	2253	5MU	O4-C4-N3	-3.40	113.60	120.12
1	1	966	2MG	C5-C6-N1	3.38	119.91	113.95
1	1	4058	OMU	O2-C2-N3	-3.37	115.22	121.50
1	1	2461	PSU	C4-N3-C2	-3.36	121.50	126.34
1	1	3423	PSU	C4-N3-C2	-3.34	121.53	126.34
1	1	2251	1MG	C5'-C4'-C3'	3.32	127.61	115.18
1	1	4009	2MA	C8-N7-C5	3.26	109.20	102.99
1	1	527	7MG	C6-C5-N7	3.26	137.03	131.91
1	1	4010	PSU	C4-N3-C2	-3.21	121.71	126.34
1	1	2251	1MG	O3'-C3'-C2'	3.17	122.09	111.82
1	1	1402	4OC	O2-C2-N1	3.15	125.40	118.89
1	1	3575	G7M	O6-C6-N1	-3.13	116.95	120.65
1	1	2251	1MG	O2'-C2'-C1'	3.11	122.32	110.85
1	1	2251	1MG	C8-N7-C5	3.08	108.86	102.99
1	1	2253	5MU	C5-C6-N1	-3.08	120.17	123.34
1	1	2252	PSU	C6-N1-C2	-3.07	119.55	122.68
1	1	2461	PSU	C6-N1-C2	-3.04	119.57	122.68
1	1	3423	PSU	C6-N1-C2	-3.02	119.59	122.68
1	1	3757	OMG	C2-N1-C6	-3.01	119.55	125.10
1	1	4058	OMU	C1'-N1-C6	-2.97	114.36	120.84
1	1	2252	PSU	C6-C5-C4	-2.97	116.12	118.20
1	1	3963	PSU	C6-C5-C4	-2.97	116.12	118.20
44	q	89	0TD	OD1-CG-CB	-2.95	116.25	122.44
1	1	3417	PSU	C6-C5-C4	-2.94	116.14	118.20
1	1	4004	OMC	C5-C6-N1	2.94	126.73	121.81
1	1	516	PSU	O4-C4-N3	-2.92	114.52	120.12
1	1	527	7MG	C6-C5-C4	-2.89	116.65	122.62
1	1	2251	1MG	O4'-C4'-C5'	2.81	118.63	109.37
1	1	3468	5MC	O2-C2-N3	-2.81	117.76	122.33
1	1	4086	PSU	C6-C5-C4	-2.79	116.25	118.20
1	1	3963	PSU	C6-N1-C2	-2.77	119.85	122.68
1	1	4058	OMU	O4-C4-C5	-2.76	120.30	125.16
1	1	4432	2MG	C8-N7-C5	2.74	108.22	102.99
1	1	3445	5MU	O2-C2-N1	-2.73	119.16	122.79
1	1	4010	PSU	C6-N1-C2	-2.69	119.94	122.68
1	1	1402	4OC	CM4-N4-C4	-2.67	117.23	122.45
1	1	1402	4OC	O4'-C1'-N1	2.67	114.46	108.36
1	1	3468	5MC	C5-C4-N3	-2.67	118.80	121.67
1	1	3421	3TD	C4-N3-C2	-2.66	121.72	124.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3124	6MZ	C4-C5-N7	-2.64	106.65	109.40
1	1	966	2MG	C8-N7-C5	2.64	108.02	102.99
1	1	516	PSU	O2-C2-N3	-2.64	116.84	121.82
1	1	1207	2MG	C8-N7-C5	2.59	107.93	102.99
1	1	3124	6MZ	C1'-N9-C4	2.56	131.14	126.64
1	1	3951	2MG	C8-N7-C5	2.56	107.86	102.99
1	1	3468	5MC	N1-C2-N3	2.55	123.44	118.81
1	1	3536	6MZ	O3'-C3'-C2'	2.53	120.01	111.82
1	1	4004	OMC	C1'-N1-C2	2.53	124.06	118.42
1	1	4086	PSU	O3'-C3'-C4'	2.52	118.32	111.05
1	1	2251	1MG	C5-C6-N1	2.48	117.64	113.90
1	1	3575	G7M	C2-N1-C6	-2.48	120.53	125.10
1	1	527	7MG	O4'-C1'-N9	-2.43	105.98	109.30
1	1	3341	2MG	CM2-N2-C2	-2.42	118.52	123.86
1	1	3341	2MG	C8-N7-C5	2.41	107.58	102.99
1	1	2251	1MG	O4'-C1'-C2'	2.40	110.43	106.93
1	1	1207	2MG	CM2-N2-C2	-2.39	118.59	123.86
1	1	4004	OMC	C4-N3-C2	2.36	124.06	120.25
1	1	966	2MG	O6-C6-C5	-2.35	119.78	124.37
1	1	4004	OMC	O3'-C3'-C2'	2.31	117.72	111.17
1	1	4058	OMU	O3'-C3'-C2'	2.31	117.72	111.17
1	1	527	7MG	O6-C6-C5	-2.31	121.88	127.54
1	1	527	7MG	C2-N1-C6	-2.30	120.91	125.10
1	1	4414	UR3	C5-C6-N1	-2.30	117.96	121.81
1	1	1402	4OC	C3'-C2'-C1'	-2.29	98.58	102.89
1	1	2253	5MU	C2'-C1'-N1	2.28	119.68	113.22
44	q	89	0TD	OD2-CG-OD1	-2.28	118.92	124.09
1	1	1407	5MC	C5-C4-N3	-2.27	119.23	121.67
1	1	3423	PSU	C6-C5-C4	-2.23	116.64	118.20
1	1	4432	2MG	CM2-N2-C2	-2.23	118.94	123.86
1	1	4086	PSU	O3'-C3'-C2'	2.20	118.93	111.82
1	1	4414	UR3	C3U-N3-C2	2.19	121.14	117.31
1	1	1402	4OC	C5-C4-N3	-2.17	119.11	122.59
1	1	3757	OMG	C8-N7-C5	2.16	107.11	102.99
1	1	4058	OMU	C5'-C4'-C3'	2.12	123.14	115.18
1	1	967	5MC	C1'-N1-C6	-2.12	117.60	121.12
1	1	3951	2MG	O6-C6-C5	-2.11	120.24	124.37
1	1	2253	5MU	O4-C4-C5	2.11	127.35	124.90
1	1	4058	OMU	CM2-O2'-C2'	-2.08	109.06	114.52
1	1	967	5MC	C5-C4-N3	-2.06	119.45	121.67
1	1	4004	OMC	C6-C5-C4	-2.06	114.19	117.50
1	1	4086	PSU	C6-N1-C2	-2.06	120.58	122.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	4434	MA6	C9-N6-C6	2.03	125.65	119.51
1	1	4058	OMU	C6-C5-C4	-2.02	116.76	119.52
1	1	3341	2MG	O6-C6-C5	-2.01	120.45	124.37
1	1	4004	OMC	O3'-C3'-C4'	2.00	116.84	111.05

All (39) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	516	PSU	C3'
1	1	516	PSU	C4'
1	1	527	7MG	C3'
1	1	1402	4OC	C1'
1	1	1402	4OC	C3'
1	1	2251	1MG	C2'
1	1	2251	1MG	C1'
1	1	2252	PSU	C3'
1	1	2252	PSU	C4'
1	1	2253	5MU	C2'
1	1	2253	5MU	C4'
1	1	2461	PSU	C3'
1	1	2461	PSU	C4'
1	1	3124	6MZ	C2'
1	1	3124	6MZ	C3'
1	1	3417	PSU	C3'
1	1	3417	PSU	C4'
1	1	3421	3TD	C3'
1	1	3423	PSU	C3'
1	1	3423	PSU	C4'
1	1	3445	5MU	C2'
1	1	3445	5MU	C4'
1	1	3536	6MZ	C2'
1	1	3536	6MZ	C3'
1	1	3575	G7M	C2'
1	1	3757	OMG	C2'
1	1	3963	PSU	C3'
1	1	3963	PSU	C4'
1	1	4004	OMC	C4'
1	1	4009	2MA	C2'
1	1	4009	2MA	C3'
1	1	4010	PSU	C3'
1	1	4010	PSU	C4'
1	1	4058	OMU	C2'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
1	1	4058	OMU	C3'
1	1	4086	PSU	C3'
1	1	4086	PSU	C4'
1	1	4111	PSU	C3'
1	1	4111	PSU	C4'

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	516	PSU	O4'-C1'-C5-C4
1	1	516	PSU	O4'-C1'-C5-C6
1	1	516	PSU	C3'-C4'-C5'-O5'
1	1	516	PSU	O4'-C4'-C5'-O5'
1	1	527	7MG	C3'-C4'-C5'-O5'
1	1	966	2MG	O4'-C4'-C5'-O5'
1	1	966	2MG	C3'-C4'-C5'-O5'
1	1	966	2MG	N1-C2-N2-CM2
1	1	966	2MG	N3-C2-N2-CM2
1	1	1402	4OC	O4'-C4'-C5'-O5'
1	1	2253	5MU	C3'-C4'-C5'-O5'
1	1	2253	5MU	O4'-C4'-C5'-O5'
1	1	3124	6MZ	N1-C6-N6-C9
1	1	3124	6MZ	O4'-C4'-C5'-O5'
1	1	3124	6MZ	C3'-C4'-C5'-O5'
1	1	3417	PSU	C3'-C4'-C5'-O5'
1	1	3421	3TD	O4'-C1'-C5-C4
1	1	3421	3TD	O4'-C1'-C5-C6
1	1	3421	3TD	C3'-C4'-C5'-O5'
1	1	3421	3TD	O4'-C4'-C5'-O5'
1	1	3423	PSU	C3'-C4'-C5'-O5'
1	1	3536	6MZ	O4'-C4'-C5'-O5'
1	1	3536	6MZ	C3'-C4'-C5'-O5'
1	1	3963	PSU	C3'-C4'-C5'-O5'
1	1	4004	OMC	C3'-C4'-C5'-O5'
1	1	4004	OMC	C4'-C5'-O5'-P
1	1	4009	2MA	O4'-C4'-C5'-O5'
1	1	4009	2MA	C3'-C4'-C5'-O5'
1	1	4058	OMU	O4'-C4'-C5'-O5'
1	1	4086	PSU	C3'-C4'-C5'-O5'
1	1	4111	PSU	C3'-C4'-C5'-O5'
1	1	4111	PSU	O4'-C4'-C5'-O5'
44	q	89	0TD	CG-CB-SB-CSB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	1	1402	4OC	C2'-C1'-N1-C2
1	1	2461	PSU	C4'-C5'-O5'-P
1	1	1402	4OC	C3'-C4'-C5'-O5'
1	1	4058	OMU	C3'-C4'-C5'-O5'
1	1	1402	4OC	C2'-C1'-N1-C6
1	1	527	7MG	O4'-C4'-C5'-O5'
1	1	3417	PSU	O4'-C4'-C5'-O5'
1	1	3963	PSU	O4'-C4'-C5'-O5'
1	1	4010	PSU	O4'-C4'-C5'-O5'
1	1	4086	PSU	O4'-C4'-C5'-O5'
1	1	4435	MA6	O4'-C4'-C5'-O5'
1	1	4010	PSU	C3'-C4'-C5'-O5'
1	1	3417	PSU	C4'-C5'-O5'-P
1	1	3423	PSU	C4'-C5'-O5'-P
1	1	3445	5MU	C4'-C5'-O5'-P
1	1	3423	PSU	O4'-C4'-C5'-O5'
1	1	4004	OMC	O4'-C4'-C5'-O5'
1	1	527	7MG	C4'-C5'-O5'-P
1	1	3963	PSU	C4'-C5'-O5'-P
1	1	4111	PSU	C4'-C5'-O5'-P
1	1	4435	MA6	C3'-C4'-C5'-O5'
1	1	516	PSU	C4'-C5'-O5'-P
1	1	2253	5MU	C4'-C5'-O5'-P
1	1	3124	6MZ	C5-C6-N6-C9
1	1	2251	1MG	C4'-C5'-O5'-P
1	1	4058	OMU	C4'-C5'-O5'-P
1	1	2461	PSU	C3'-C4'-C5'-O5'
1	1	3124	6MZ	C4'-C5'-O5'-P
1	1	3757	OMG	O4'-C4'-C5'-O5'
1	1	4010	PSU	C4'-C5'-O5'-P
1	1	4086	PSU	C4'-C5'-O5'-P
1	1	3575	G7M	C4'-C5'-O5'-P
1	1	2252	PSU	O4'-C1'-C5-C4
1	1	2253	5MU	C2'-C1'-N1-C6
1	1	4435	MA6	C5-C6-N6-C10
1	1	2461	PSU	O4'-C4'-C5'-O5'
1	1	4434	MA6	O4'-C4'-C5'-O5'
1	1	2252	PSU	O4'-C1'-C5-C6
1	1	2252	PSU	C3'-C4'-C5'-O5'
1	1	3575	G7M	O4'-C4'-C5'-O5'
1	1	3757	OMG	C3'-C4'-C5'-O5'
1	1	2253	5MU	C2'-C1'-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	1	4004	OMC	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 438 ligands modelled in this entry, 438 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1501:U	O3'	1502:U	P	3.88
1	1	1276:G	O3'	1277:C	P	3.82
1	1	3820:A	O3'	3821:G	P	3.74

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1383:C	O3'	1384:C	P	3.50
1	1	147:G	O3'	148:G	P	3.31

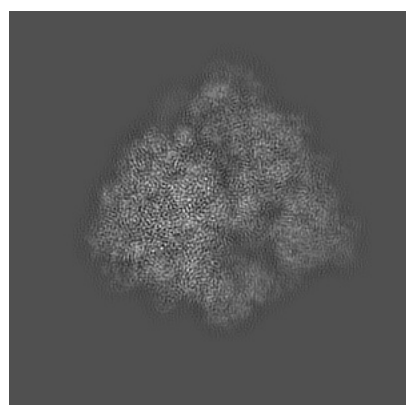
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0261. These allow visual inspection of the internal detail of the map and identification of artifacts.

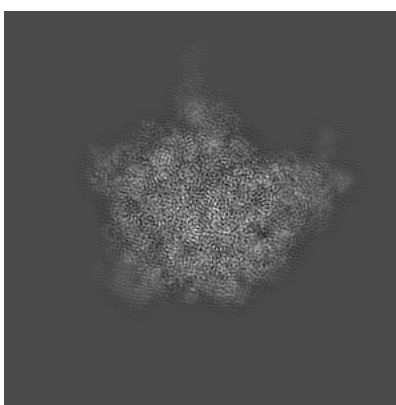
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

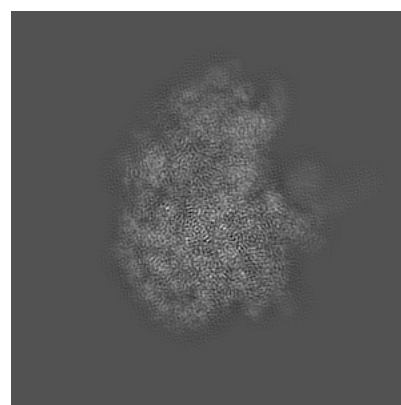
6.1.1 Primary map



X



Y

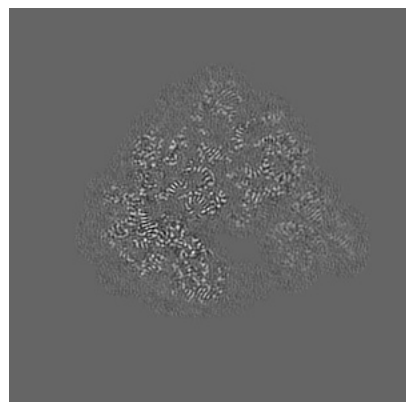


Z

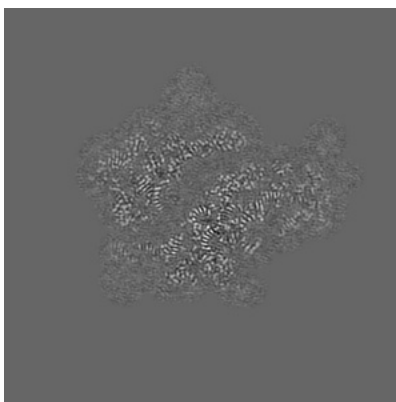
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

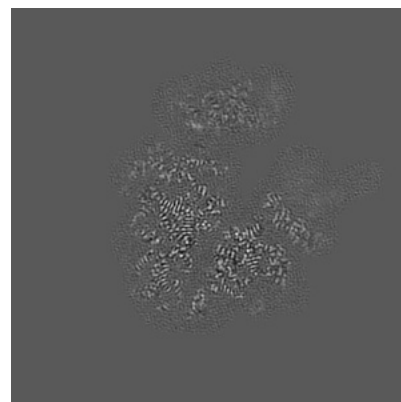
6.2.1 Primary map



X Index: 185



Y Index: 185

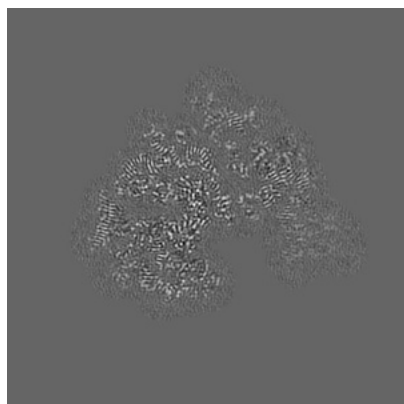


Z Index: 185

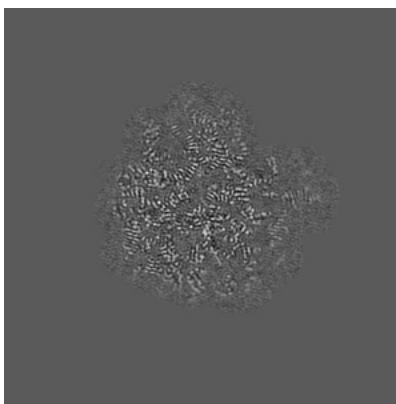
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

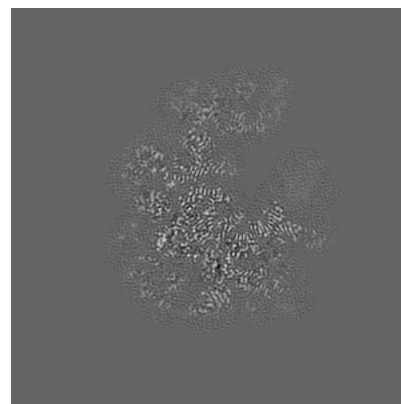
6.3.1 Primary map



X Index: 175



Y Index: 168



Z Index: 194

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

6.4 Orthogonal surface views [i](#)

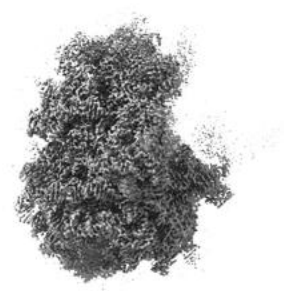
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

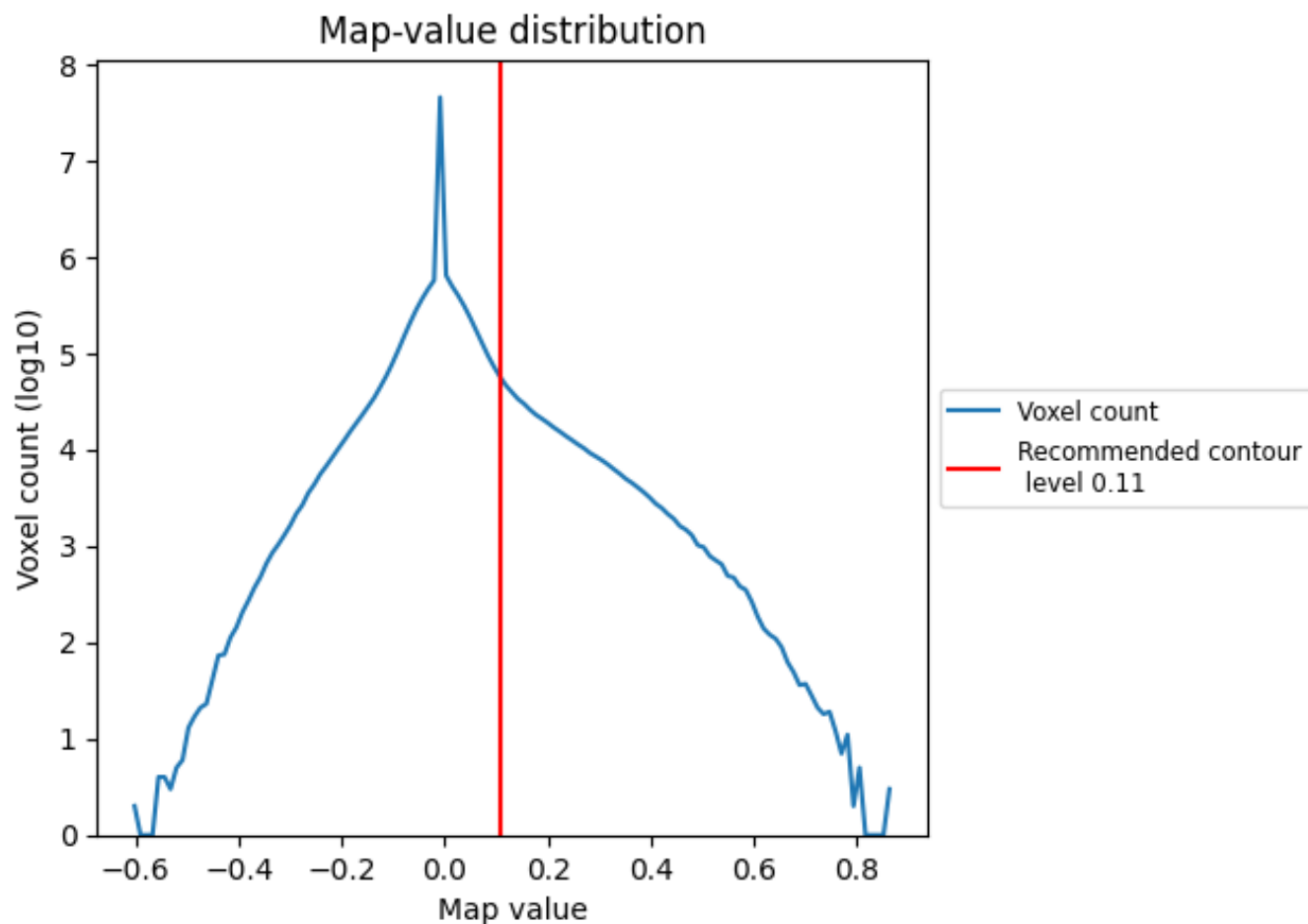
6.5 Mask visualisation

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

7 Map analysis [i](#)

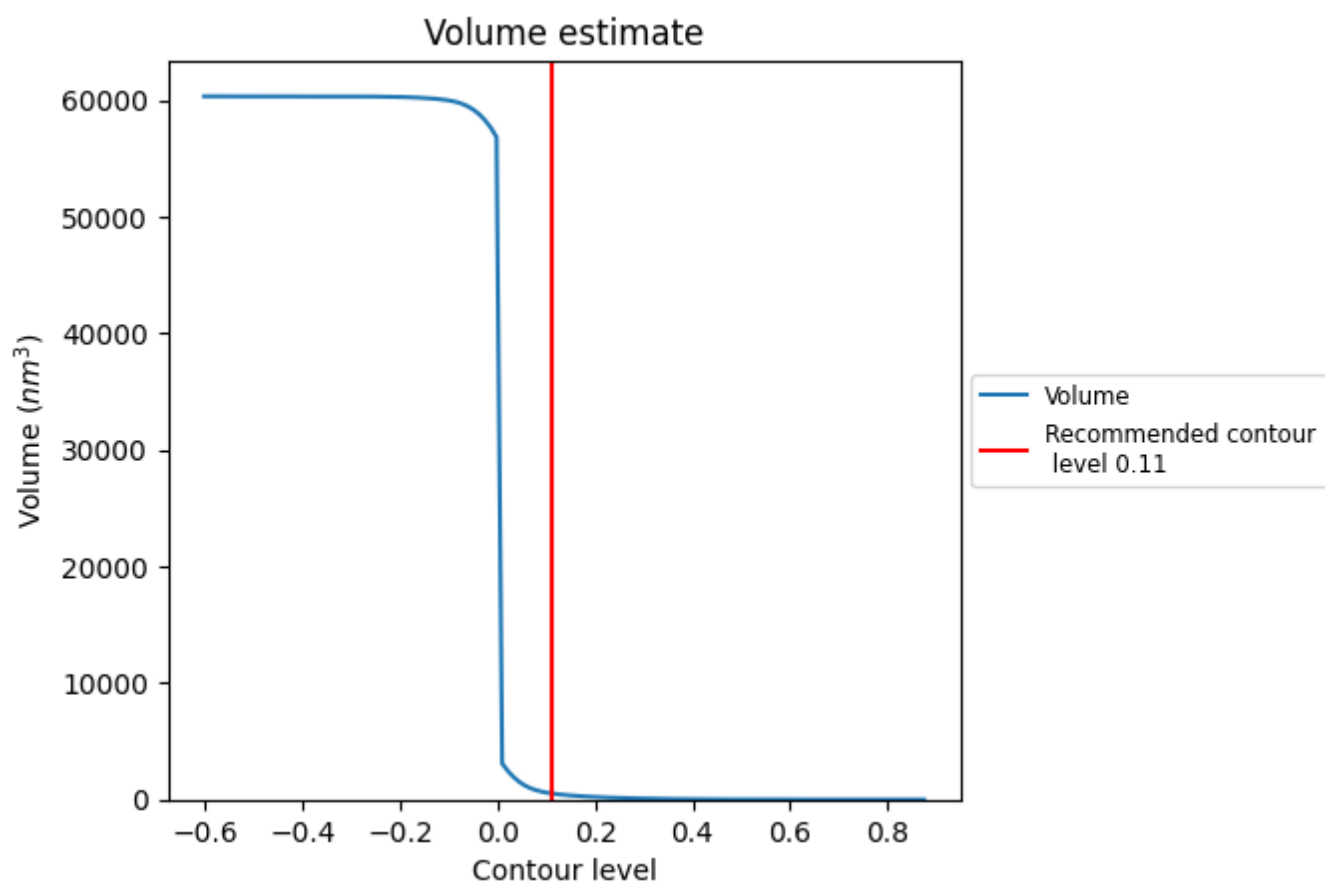
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

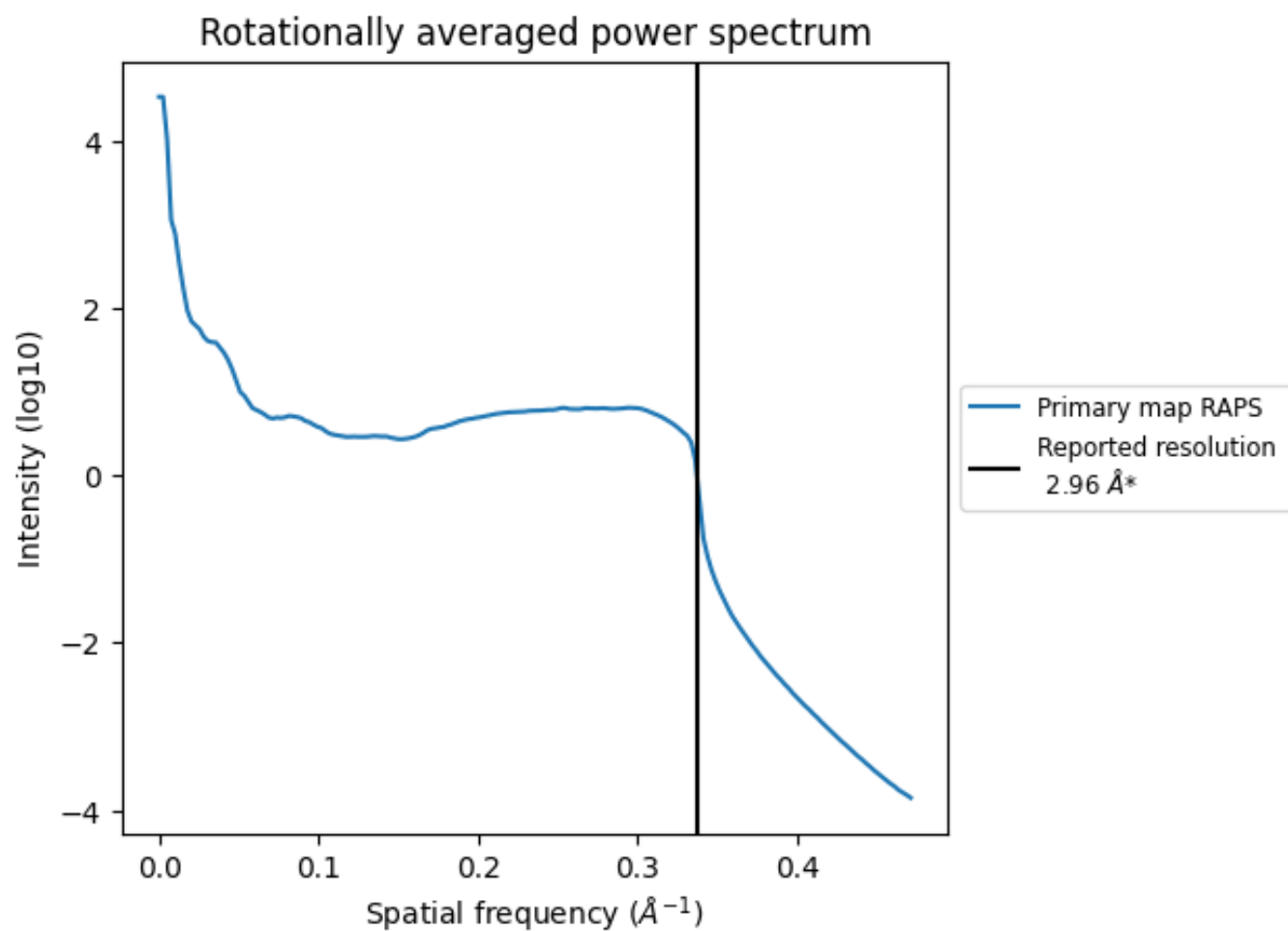
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 532 nm³; this corresponds to an approximate mass of 480 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 ⓘ

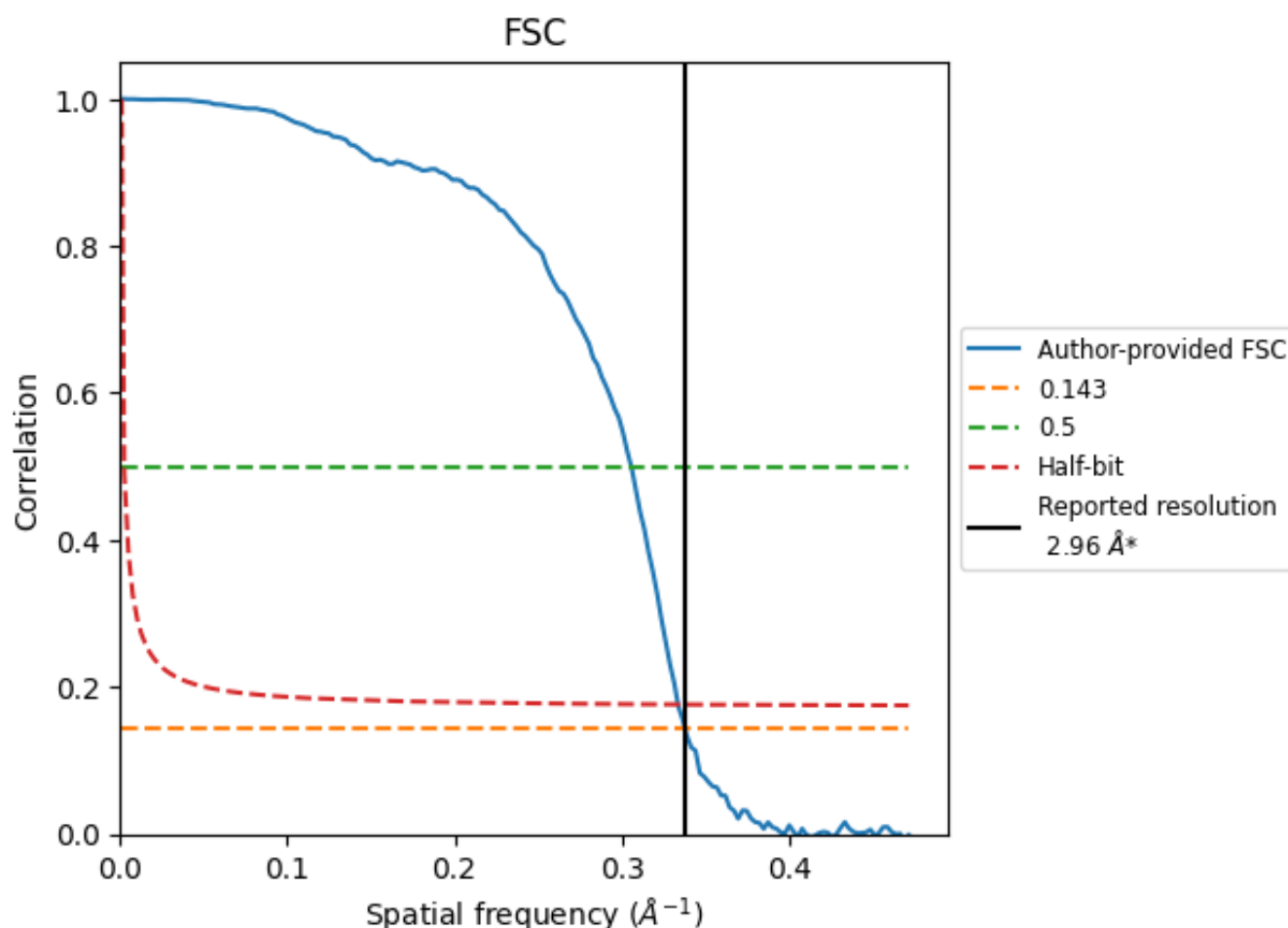


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

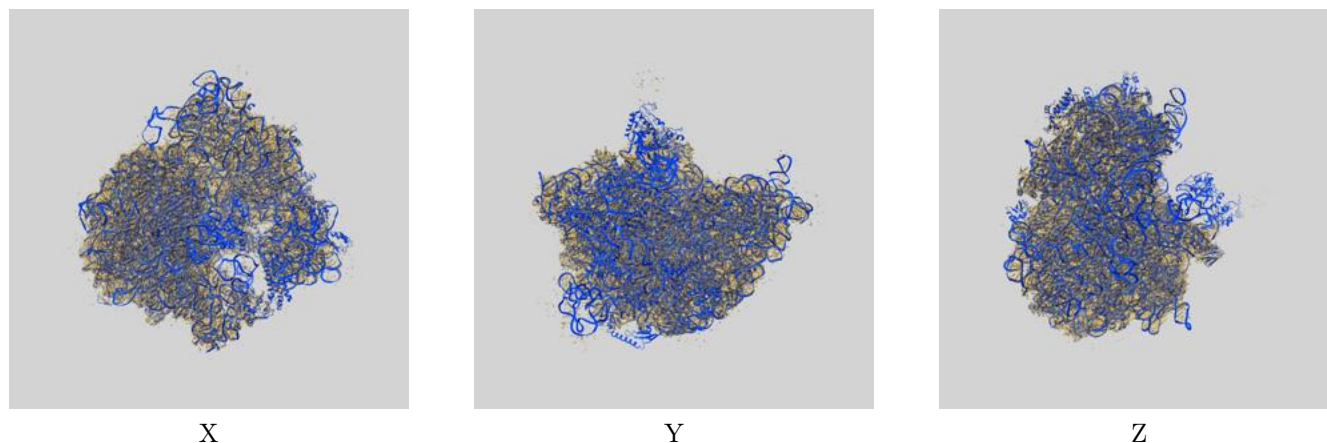
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.27	3.00
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

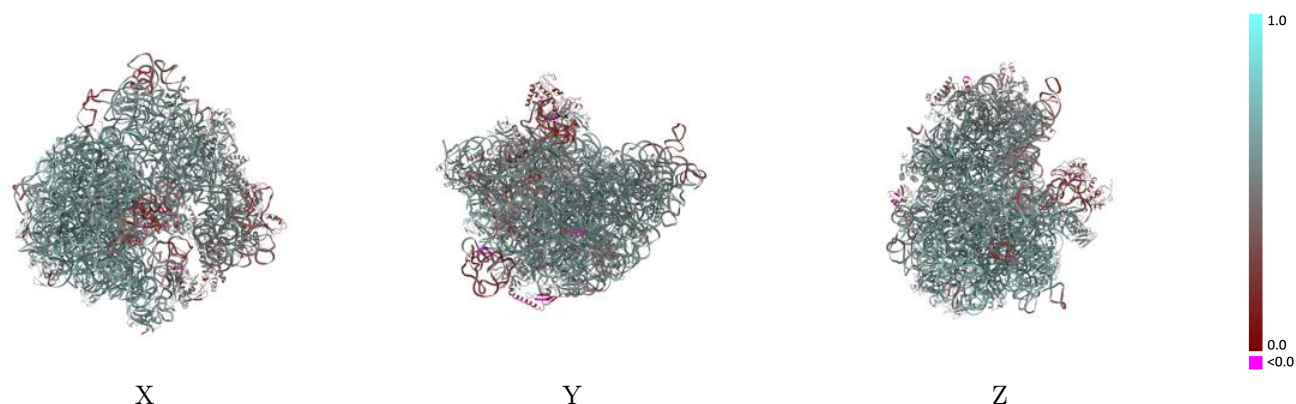
This section contains information regarding the fit between EMDB map EMD-0261 and PDB model 6HRM. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



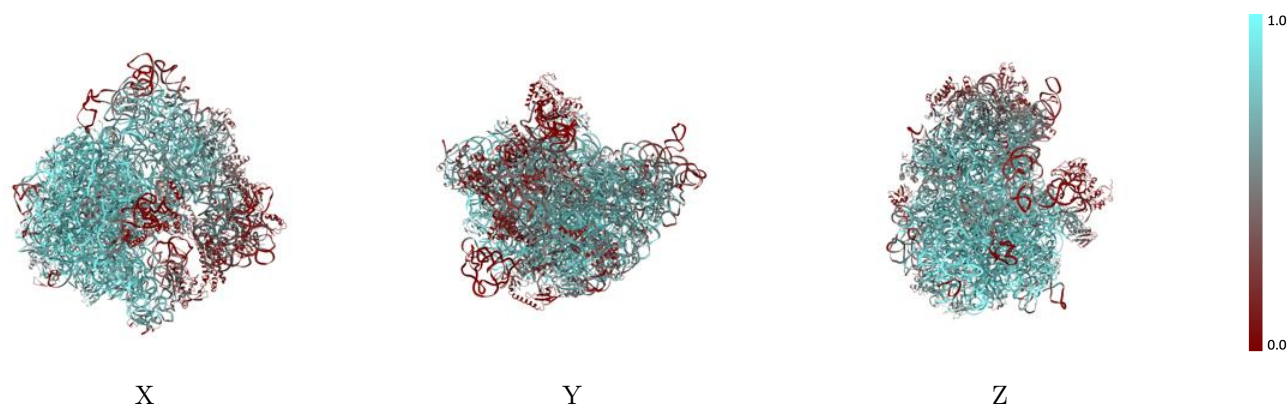
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



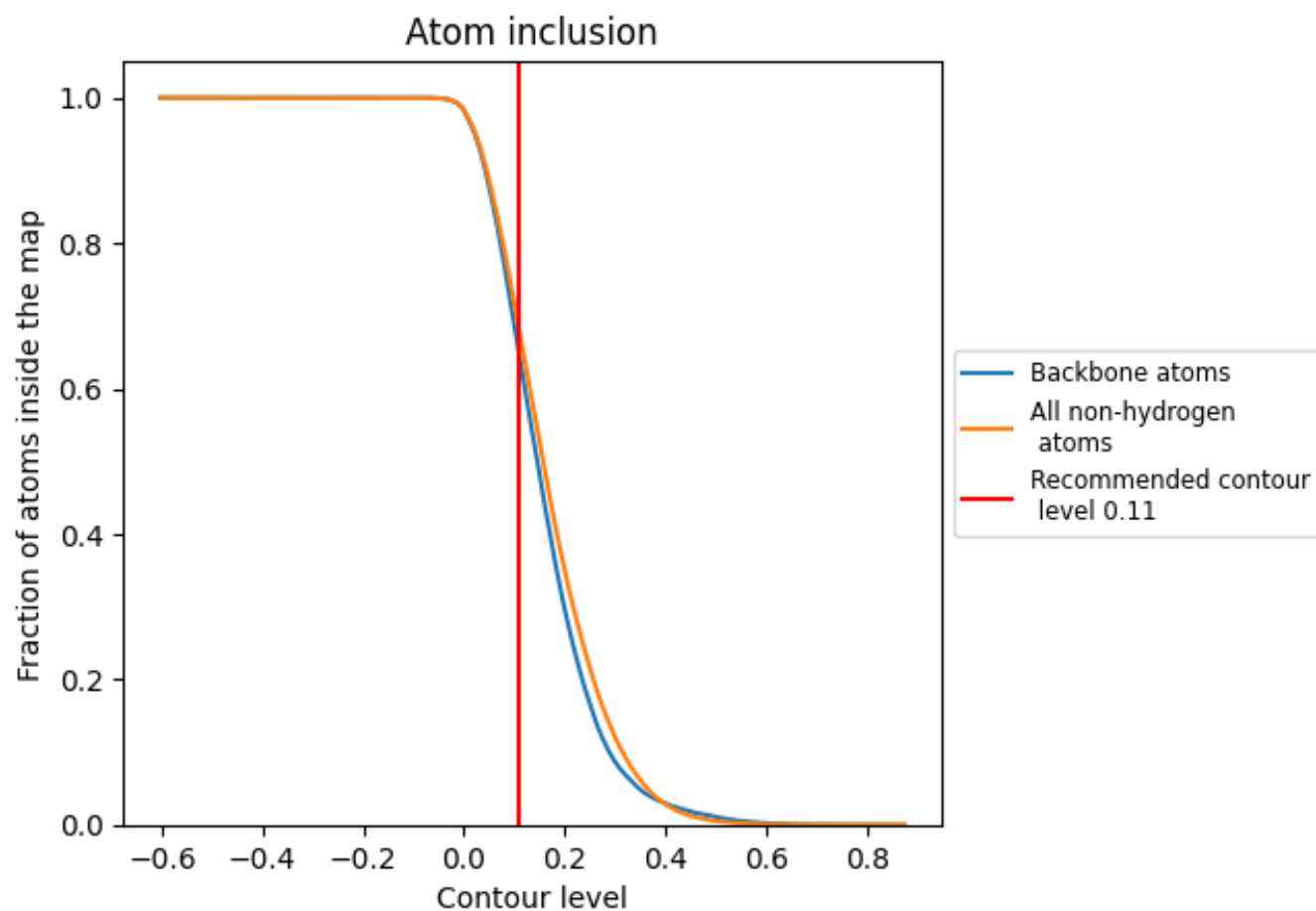
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 68% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6796	 0.5570
1	 0.7540	 0.5750
3	 0.7284	 0.5840
B	 0.8468	 0.6190
C	 0.7978	 0.6040
D	 0.6461	 0.5600
E	 0.2809	 0.4640
F	 0.4600	 0.5240
G	 0.1186	 0.2870
H	 0.0073	 0.2210
I	 0.0031	 0.2590
J	 0.7964	 0.6100
K	 0.7948	 0.6010
L	 0.7539	 0.5920
M	 0.7697	 0.5990
N	 0.8370	 0.6130
O	 0.6141	 0.5590
P	 0.7447	 0.5980
Q	 0.8240	 0.6160
R	 0.7240	 0.5830
S	 0.7667	 0.6060
T	 0.6753	 0.5670
U	 0.5508	 0.5240
V	 0.6477	 0.5690
W	 0.7968	 0.6160
X	 0.7637	 0.6030
Y	 0.4969	 0.5300
Z	 0.7477	 0.5870
a	 0.1230	 0.3660
b	 0.7576	 0.6050
c	 0.6914	 0.5810
d	 0.8620	 0.6100
e	 0.8350	 0.6260
f	 0.7816	 0.5930
g	 0.2603	 0.4290



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
h	 0.3516	 0.4760
i	 0.4217	 0.4960
j	 0.5735	 0.5210
k	 0.5079	 0.5170
l	 0.1844	 0.4350
m	 0.6052	 0.5470
n	 0.1951	 0.4340
o	 0.2340	 0.3990
p	 0.5252	 0.5310
q	 0.6446	 0.5530
r	 0.1843	 0.4320
s	 0.3333	 0.4810
t	 0.6319	 0.5630
u	 0.5327	 0.5260
v	 0.5134	 0.5240
w	 0.6176	 0.5470
x	 0.1515	 0.4140
y	 0.5810	 0.5540
z	 0.2326	 0.4530