Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:38 pm GMT

PDB ID	:	6Q8Y
EMDB ID	:	EMD-4474
Title	:	Cryo-EM structure of the mRNA translating and degrading yeast 80S ribosome-Xrn1 nuclease complex
Authors	:	Tesina, P.; Heckel, E.; Cheng, J.; Buschauer, R.; Kater, L.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on	:	2018-12-16
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

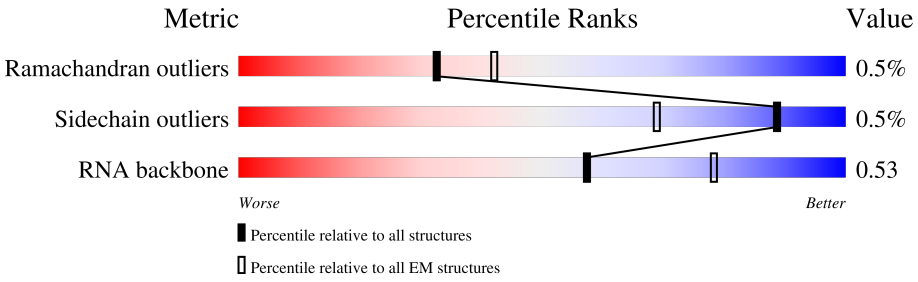
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2	1797	67% 29%
2	AA	233	97%
3	AB	136	99%
4	AC	100	94% 5%
5	AD	191	99%
6	AE	67	7% 100%
7	AF	87	98%
8	AG	169	99%

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Mol	Chain	Length	Quality of chain
9	AH	121	100%
10	AI	77	99%
11	AJ	193	95% 5%
12	AK	126	99%
13	AL	50	96%
14	AM	136	99%
15	AN	135	99%
16	AO	52	100%
17	AP	105	98%
18	AQ	203	95% 5%
19	AR	148	97%
20	AS	25	96%
21	AT	91	97%
22	AU	197	99%
23	AV	58	7% 100%
24	AW	252	96%
25	AX	183	5% 98%
26	a	87	98%
27	b	129	99%
28	c	144	97%
29	d	132	10% 97%
30	e	97	9% 91% 6%
31	f	81	100%
32	g	60	10% 100%
33	z	916	72% 93% 5%

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Mol	Chain	Length	Quality of chain
34	l	17	12% 53% 47%
35	n	76	5% 80% 20%
36	m	75	5% 72% 27%
37	AY	97	99%
38	BA	386	98%
39	BB	185	98%
40	BC	109	97%
41	BD	220	5% 98%
42	BE	361	98%
43	BF	188	97%
44	BG	127	99%
45	BH	172	100%
46	BI	296	99%
47	BJ	159	97%
48	BK	106	100%
49	BL	100	100%
50	BM	175	88% 11%
51	BN	112	98%
52	BO	222	98%
53	BP	119	93% 6%
54	BQ	3396	68% 23% 7%
55	BR	121	80% 19%
56	BS	158	72% 27%
57	A	223	99%
58	B	206	97%

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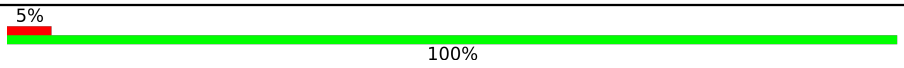
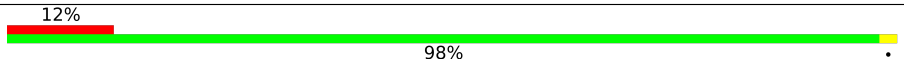
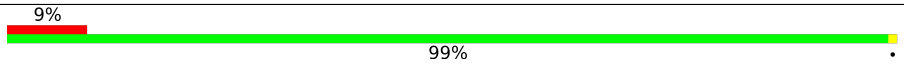
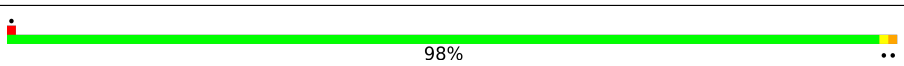
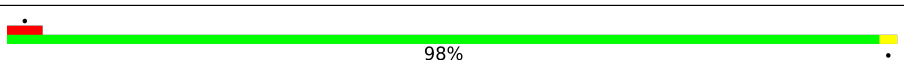
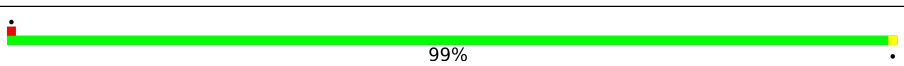
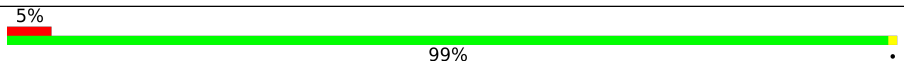
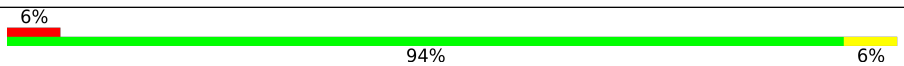
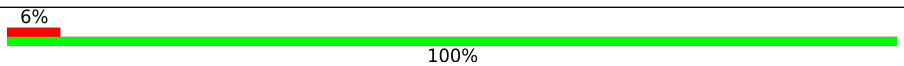
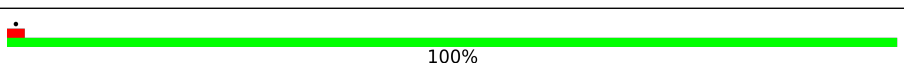
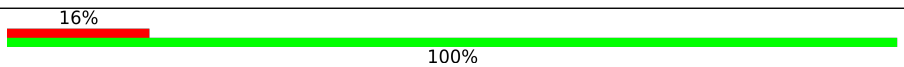
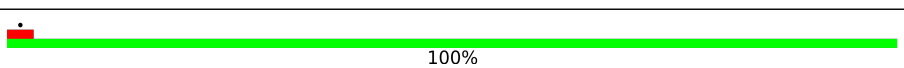
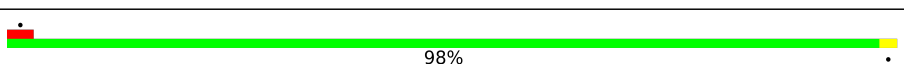
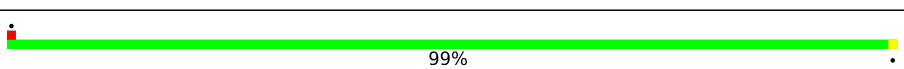
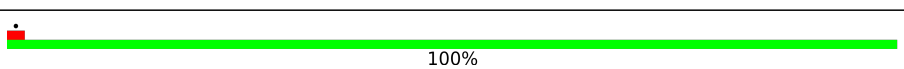
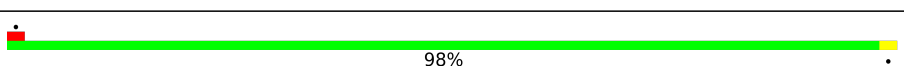
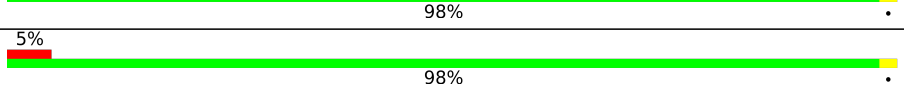
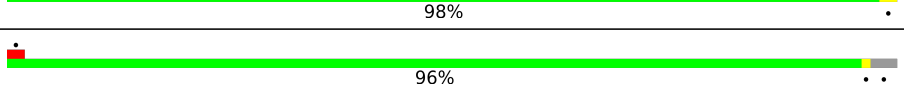
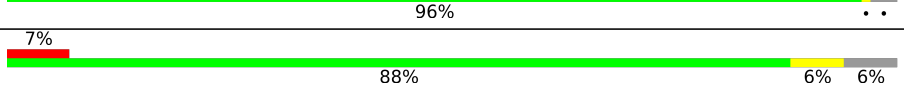
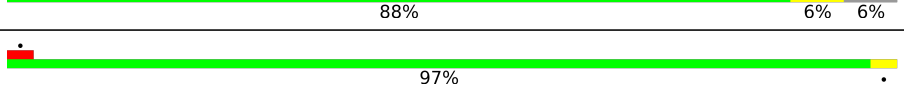
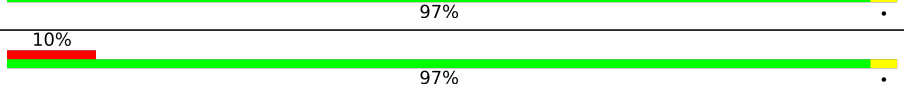
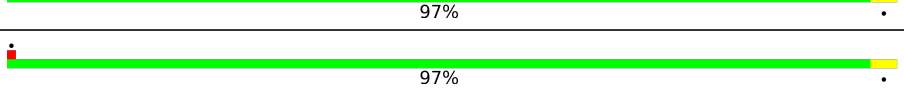
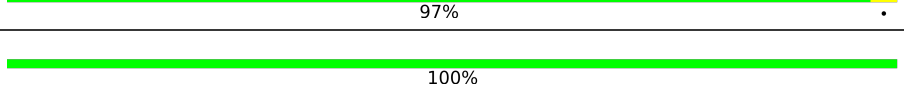
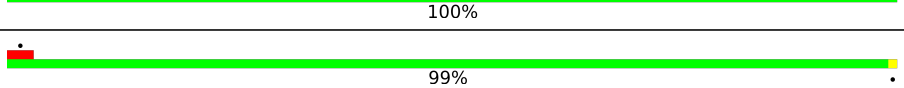
Mol	Chain	Length	Quality of chain
59	C	96	
60	D	121	
61	E	121	
62	F	141	
63	G	125	
64	H	139	
65	J	107	
66	K	70	
67	L	63	
68	M	53	
69	N	51	
70	O	318	
71	P	219	
72	Q	214	
73	R	220	
74	S	260	
75	T	226	
76	U	184	
77	V	199	
78	W	178	
79	X	155	
80	Y	150	
81	Z	127	
82	I	143	

2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 209410 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1767	37645	16830	6656	12392	1767	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1570	G	A	conflict	GB 1329886537

- Molecule 2 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AA	233	1804	1151	323	327	3	0	0

- Molecule 3 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AB	136	1003	628	189	179	7	0	0

- Molecule 4 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AC	99	771	481	156	132	2	0	0

- Molecule 5 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AD	191	1518	963	274	277	4	0	0

- Molecule 6 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AE	67	Total	C	N	O	S	0	0
			543	349	106	87	1		

- Molecule 7 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AF	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 8 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AG	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 9 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AH	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 10 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	AI	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 11 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	AJ	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 12 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	AK	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 13 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AL	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 14 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AM	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 15 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	AN	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 16 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AO	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 17 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AP	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AQ	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 19 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AR	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 20 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AS	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 21 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AT	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 22 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AU	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 23 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	AV	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 24 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AW	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 25 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	AX	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 26 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 27 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 28 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 29 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	d	132	Total	C	N	O	0	0
			1060	669	206	185		

- Molecule 30 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 31 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	60	Total	C	N	O	S	0	0
			473	297	98	77	1		

- Molecule 33 is a protein called 5'-3' exoribonuclease 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	874	Total	C	N	O	S	0	0
			7181	4639	1194	1320	28		

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	17	Total	C	N	O	P	0	0
			367	164	70	116	17		

- Molecule 35 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	76	Total	C	N	O	P	0	0
			1621	723	291	531	76		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	74	C	-	insertion	GB 1329886529
n	75	C	-	insertion	GB 1329886529
n	76	A	-	insertion	GB 1329886529

- Molecule 36 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	75	Total	C	N	O	P	0	0
			1589	710	279	525	75		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	11	C	U	conflict	GB 176418

- Molecule 37 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AY	97	Total	C	N	O	S	0	0
			742	479	124	138	1		

- Molecule 38 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BA	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 39 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BB	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 40 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BC	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 41 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BD	220	Total	C	N	O	S	0	0
			1770	1121	335	307	7		

- Molecule 42 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BE	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 43 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	BF	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 44 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BG	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 45 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BH	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 46 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BI	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 47 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BJ	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 48 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BK	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 49 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	BL	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 50 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BM	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 51 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BN	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 52 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BO	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 53 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BP	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 54 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BQ	3161	Total	C	N	O	P	0	0
			67610	30200	12186	22063	3161		

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BR	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 56 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BS	158	Total	C	N	O	P	0	0
			3352	1500	586	1108	158		

- Molecule 57 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	A	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 58 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B	206	Total	C	N	O	S	0	0
			1603	1004	297	299	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
59	C	96	Total	C	N	O	S	0	0
			813	527	133	151	2		

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	D	121	Total	C	N	O	S	0	0
			877	552	153	170	2		

- Molecule 61 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	E	121	Total	C	N	O	S	0	0
			957	611	176	163	7		

- Molecule 62 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	F	141	Total	C	N	O	0	0
			1099	704	202	193		

- Molecule 63 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	G	125	Total	C	N	O	S	0	0
			1001	625	188	186	2		

- Molecule 64 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	H	139	Total	C	N	O	S	0	0
			1143	716	222	203	2		

- Molecule 65 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	J	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 66 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	K	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 67 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	L	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 68 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	M	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 69 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	N	51	Total	C	N	O	S	0	0
			397	249	73	71	4		

- Molecule 70 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	O	318	Total	C	N	O	S	0	0
			2436	1541	418	469	8		

- Molecule 71 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	P	219	Total	C	N	O	S	0	0
			1691	1082	296	311	2		

- Molecule 72 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Q	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 73 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	R	220	Total	C	N	O	S	0	0
			1671	1072	297	300	2		

- Molecule 74 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	S	260	Total	C	N	O	S	0	0
			2061	1309	389	360	3		

- Molecule 75 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	T	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 76 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
76	U	179	Total	C	N	O	0	0
			1442	926	259	257		

- Molecule 77 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	V	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 78 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	W	178	Total	C	N	O	S	0	0
			1434	905	276	252	1		

- Molecule 79 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	X	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 80 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Y	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 81 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Z	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 82 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	I	143	Total	C	N	O	S	0	0
			1101	688	204	207	2		

- Molecule 83 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
83	AF	1	Total	Zn	0
			1	1	
83	AO	1	Total	Zn	0
			1	1	
83	AP	1	Total	Zn	0
			1	1	
83	AT	1	Total	Zn	0
			1	1	
83	e	1	Total	Zn	0
			1	1	
83	BN	1	Total	Zn	0
			1	1	
83	M	1	Total	Zn	0
			1	1	
83	N	1	Total	Zn	0
			1	1	

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

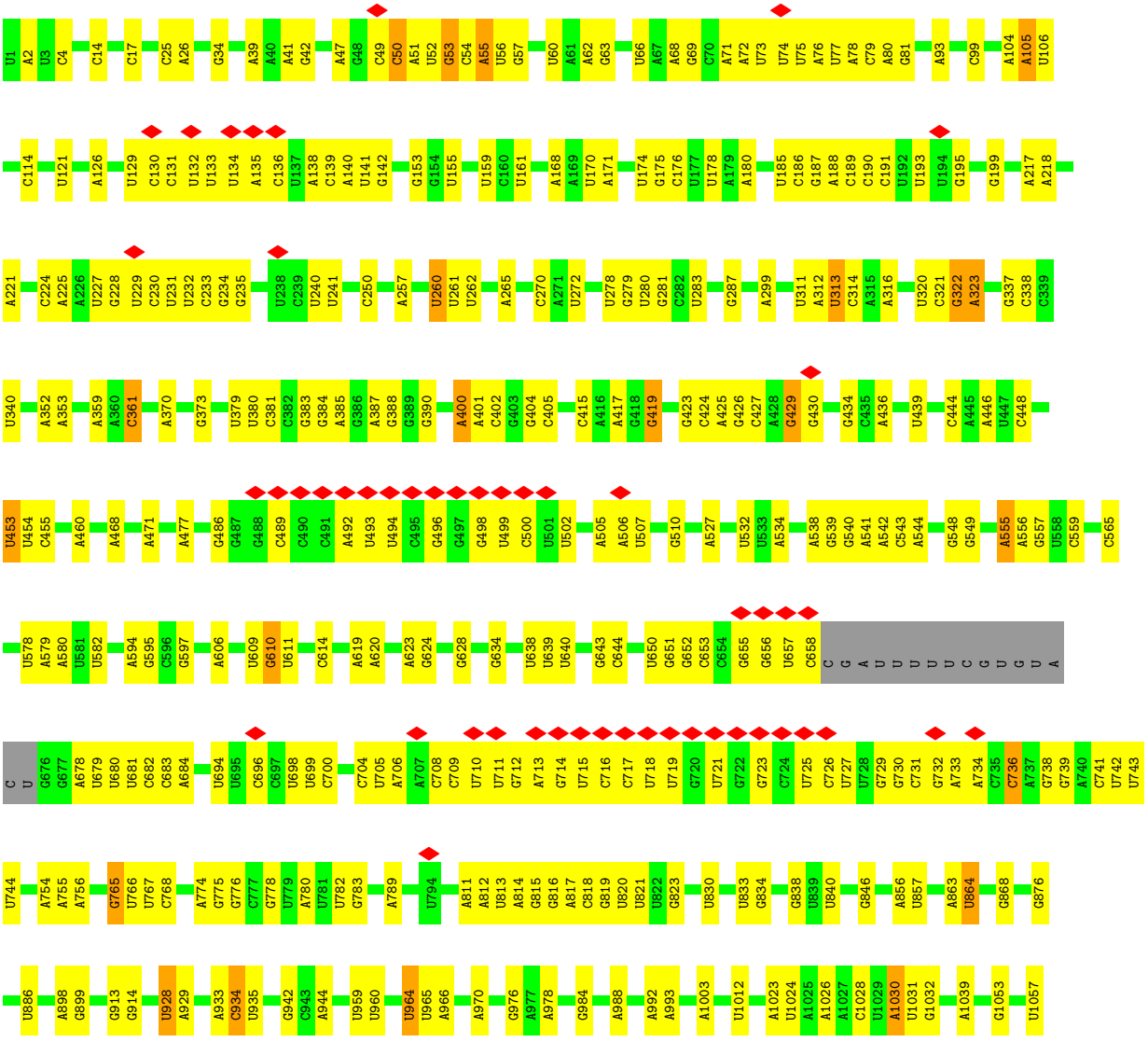
Mol	Chain	Residues	Atoms		AltConf
84	z	1	Total	Mg	0
			1	1	
84	l	1	Total	Mg	0
			1	1	

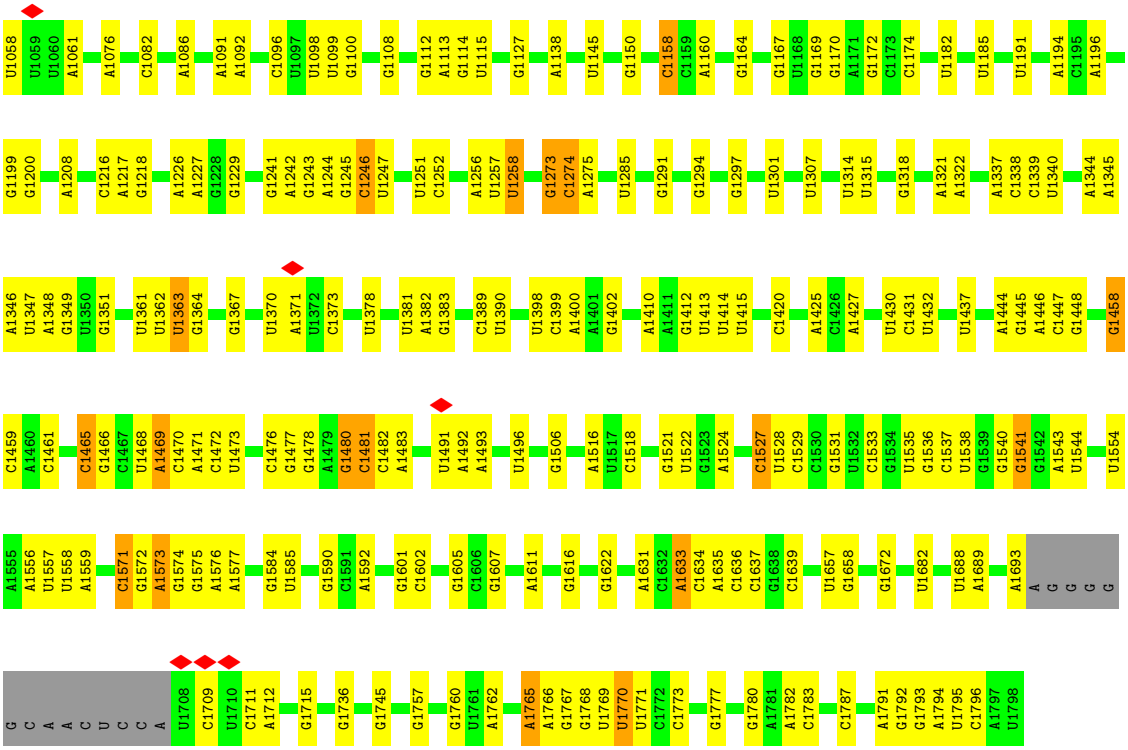
3 Residue-property plots (i)

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

- Molecule 1: 18S ribosomal RNA

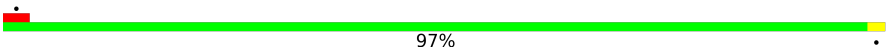
Chain 2:

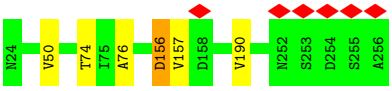




• Molecule 2: 60S ribosomal protein L8-A

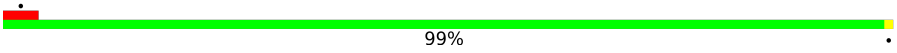
Chain AA:

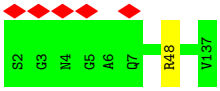




• Molecule 3: 60S ribosomal protein L23-A

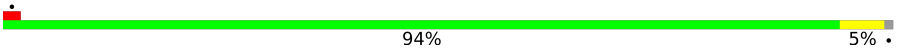
Chain AB:

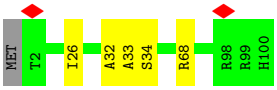




• Molecule 4: 60S ribosomal protein L36-A

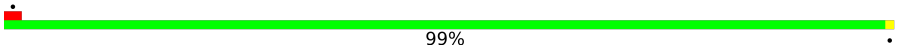
Chain AC:

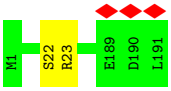




• Molecule 5: 60S ribosomal protein L9-A

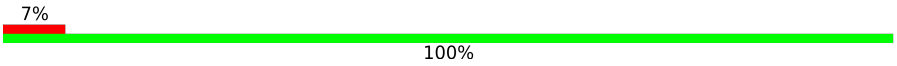
Chain AD:

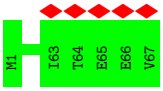




• Molecule 6: 60S ribosomal protein L24-A

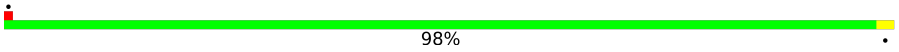
Chain AE:

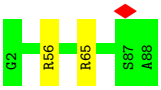




• Molecule 7: 60S ribosomal protein L37-A

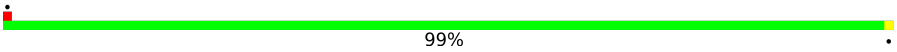
Chain AF:

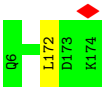




• Molecule 8: 60S ribosomal protein L11-B

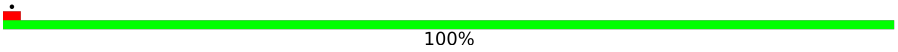
Chain AG:





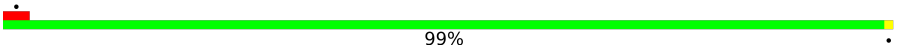
• Molecule 9: 60S ribosomal protein L25

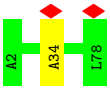
Chain AH:



• Molecule 10: 60S ribosomal protein L38

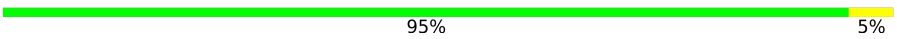
Chain AI:





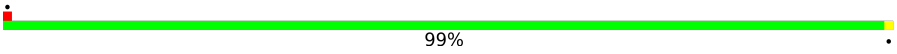
• Molecule 11: 60S ribosomal protein L13-A

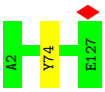
Chain AJ:



• Molecule 12: 60S ribosomal protein L26-A

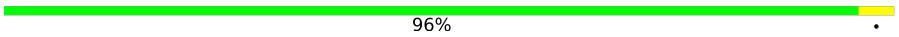
Chain AK:

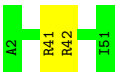




• Molecule 13: 60S ribosomal protein L39

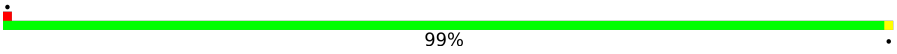
Chain AL:

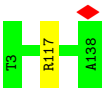




• Molecule 14: 60S ribosomal protein L14-A

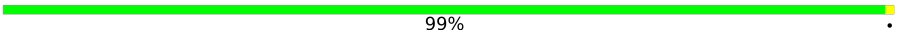
Chain AM:





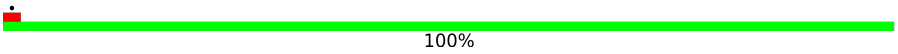
• Molecule 15: 60S ribosomal protein L27-A

Chain AN:



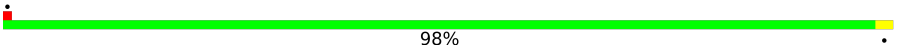
• Molecule 16: Ubiquitin-60S ribosomal protein L40

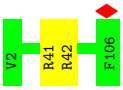
Chain AO:



• Molecule 17: 60S ribosomal protein L42-A

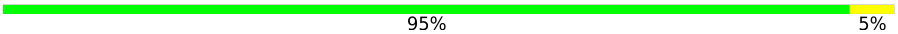
Chain AP:

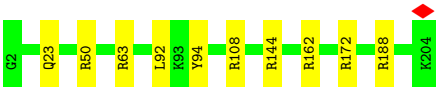




• Molecule 18: 60S ribosomal protein L15-A

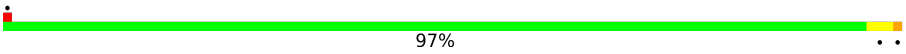
Chain AQ:

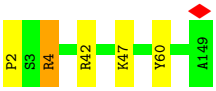




• Molecule 19: 60S ribosomal protein L28

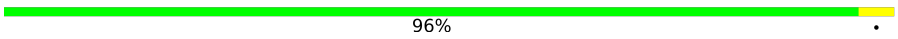
Chain AR:





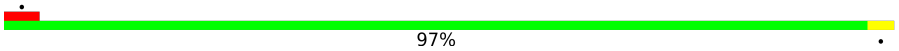
• Molecule 20: 60S ribosomal protein L41-B

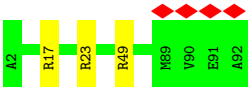
Chain AS:



• Molecule 21: 60S ribosomal protein L43-A

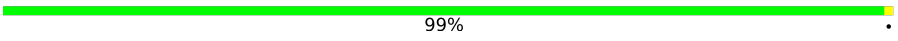
Chain AT:





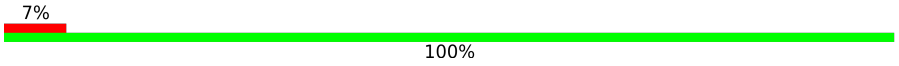
• Molecule 22: 60S ribosomal protein L16-A

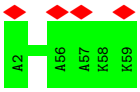
Chain AU:



• Molecule 23: 60S ribosomal protein L29

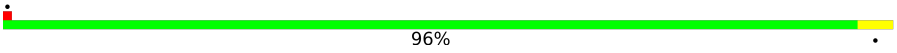
Chain AV:

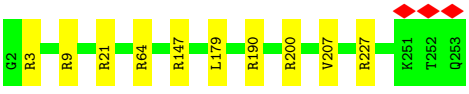




• Molecule 24: 60S ribosomal protein L2-A

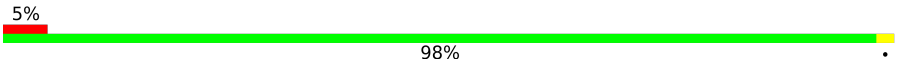
Chain AW:

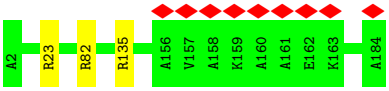




• Molecule 25: 60S ribosomal protein L17-A

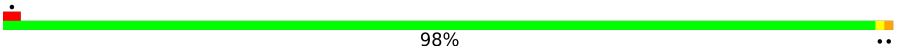
Chain AX:

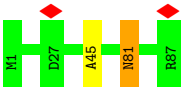




• Molecule 26: 40S ribosomal protein S21-A

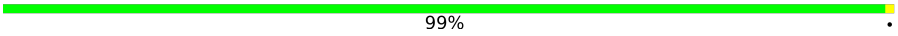
Chain a:





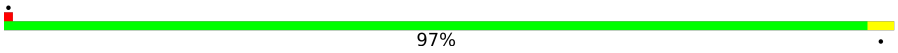
• Molecule 27: 40S ribosomal protein S22-A

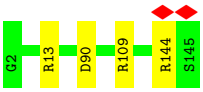
Chain b:



• Molecule 28: 40S ribosomal protein S23-A

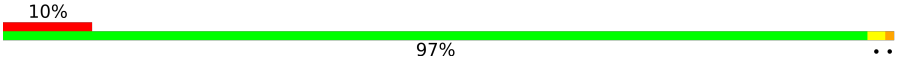
Chain c:

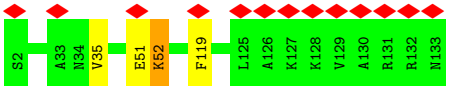




• Molecule 29: 40S ribosomal protein S24-A

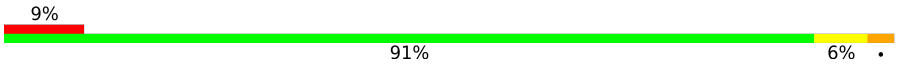
Chain d:

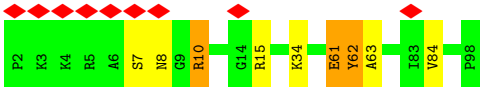




• Molecule 30: 40S ribosomal protein S26-B

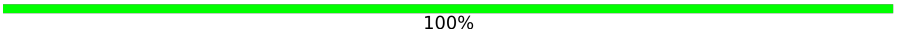
Chain e:





• Molecule 31: 40S ribosomal protein S27-A

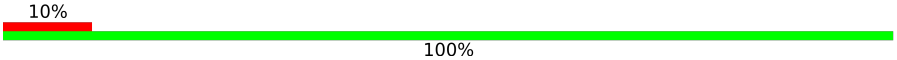
Chain f:

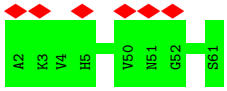


There are no outlier residues recorded for this chain.

• Molecule 32: 40S ribosomal protein S30-A

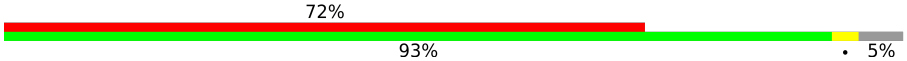
Chain g:

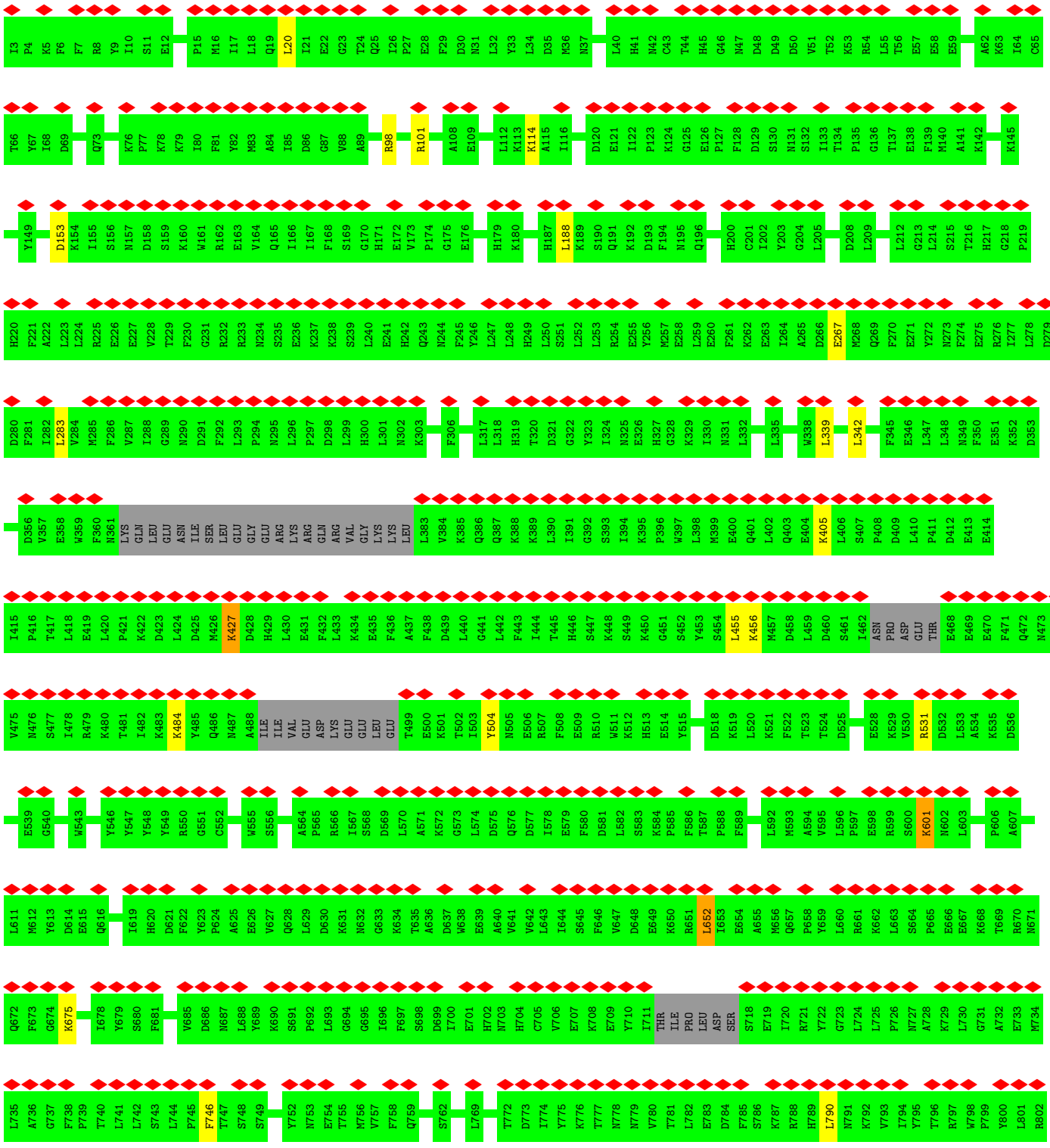


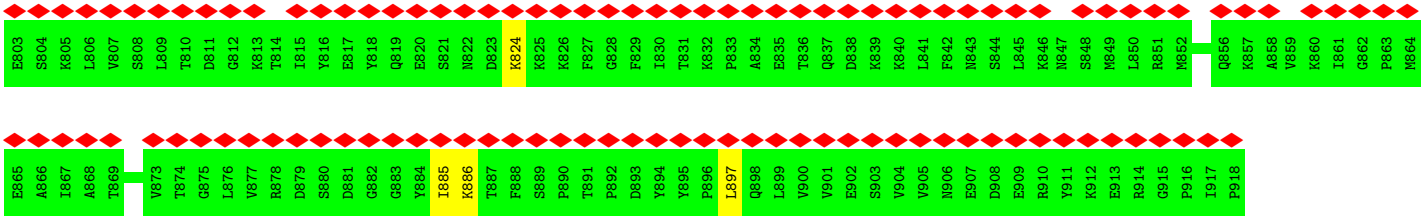


• Molecule 33: 5'-3' exoribonuclease 1

Chain z:

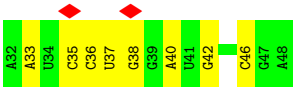






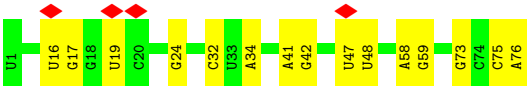
• Molecule 34: mRNA

Chain l:



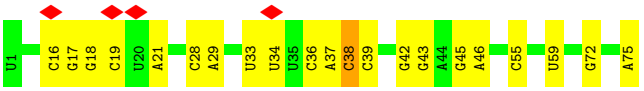
• Molecule 35: P-site tRNA

Chain n:



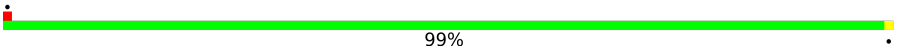
• Molecule 36: E-site tRNA

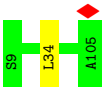
Chain m:



• Molecule 37: 60S ribosomal protein L30

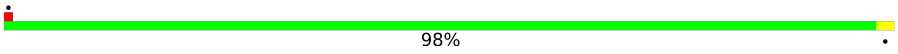
Chain AY:

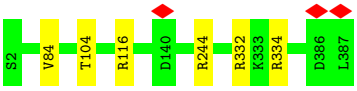




• Molecule 38: 60S ribosomal protein L3

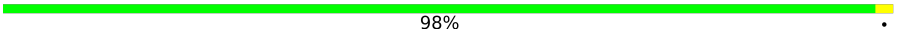
Chain BA:





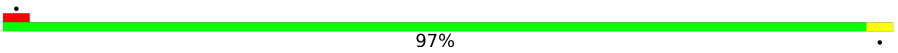
• Molecule 39: 60S ribosomal protein L18-A

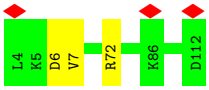
Chain BB:



• Molecule 40: 60S ribosomal protein L31-A

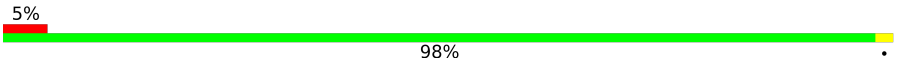
Chain BC:

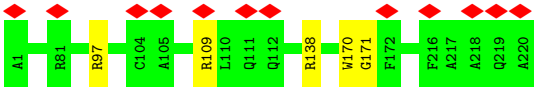




• Molecule 41: 60S ribosomal protein L10

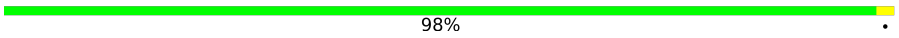
Chain BD:

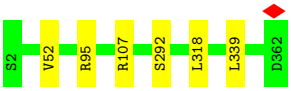




• Molecule 42: 60S ribosomal protein L4-A

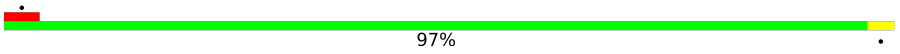
Chain BE:

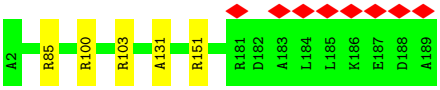




• Molecule 43: 60S ribosomal protein L19-A

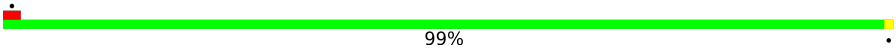
Chain BF:

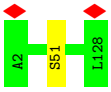




• Molecule 44: 60S ribosomal protein L32

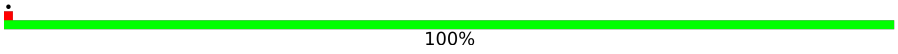
Chain BG:





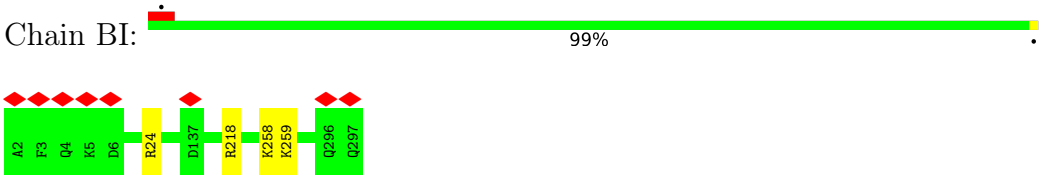
• Molecule 45: 60S ribosomal protein L20-A

Chain BH:



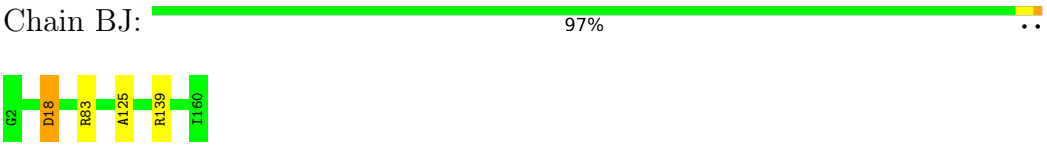
• Molecule 46: 60S ribosomal protein L5

Chain BI:



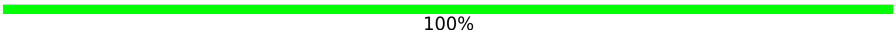
• Molecule 47: 60S ribosomal protein L21-A

Chain BJ:



• Molecule 48: 60S ribosomal protein L33-A

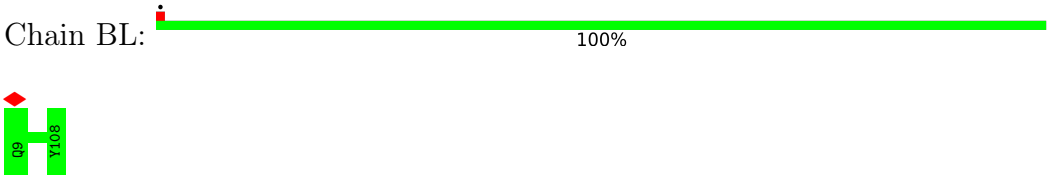
Chain BK:



There are no outlier residues recorded for this chain.

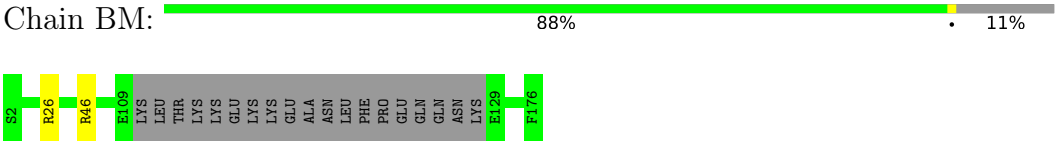
• Molecule 49: 60S ribosomal protein L22-A

Chain BL:



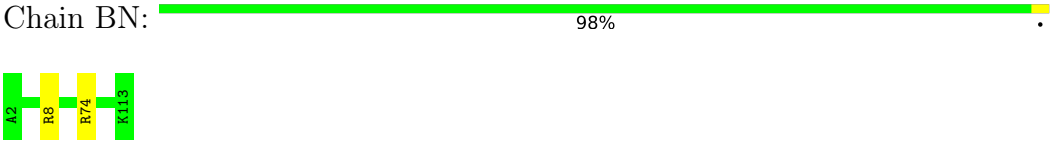
• Molecule 50: 60S ribosomal protein L6-A

Chain BM:



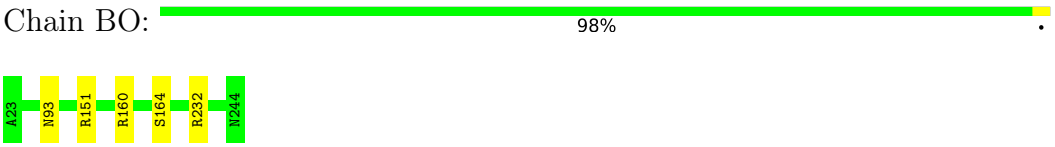
• Molecule 51: 60S ribosomal protein L34-A

Chain BN:



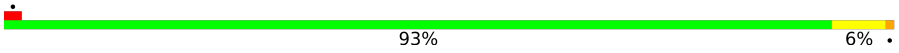
• Molecule 52: 60S ribosomal protein L7-A

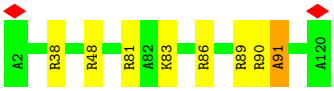
Chain BO:



• Molecule 53: 60S ribosomal protein L35-A

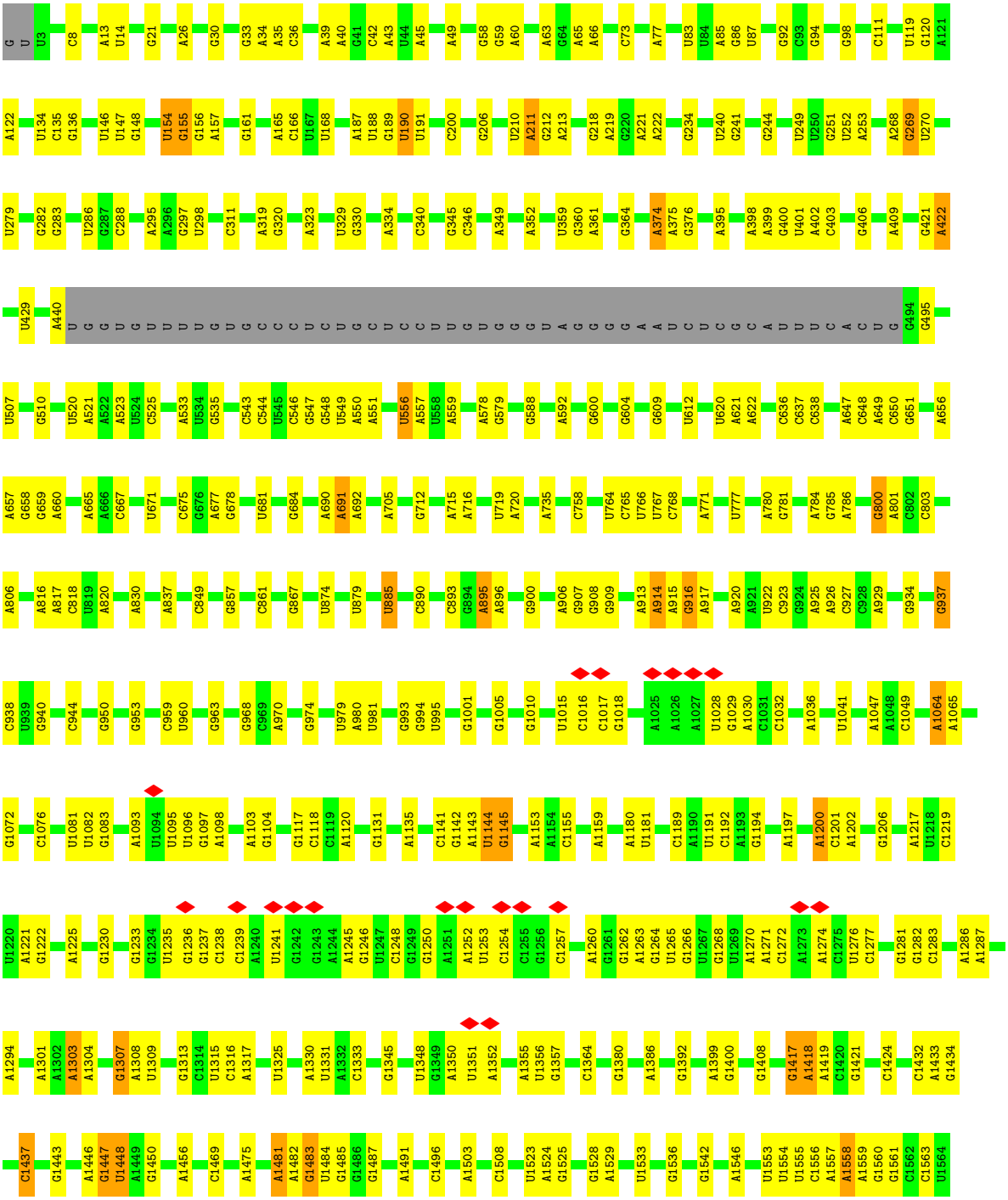
Chain BP:

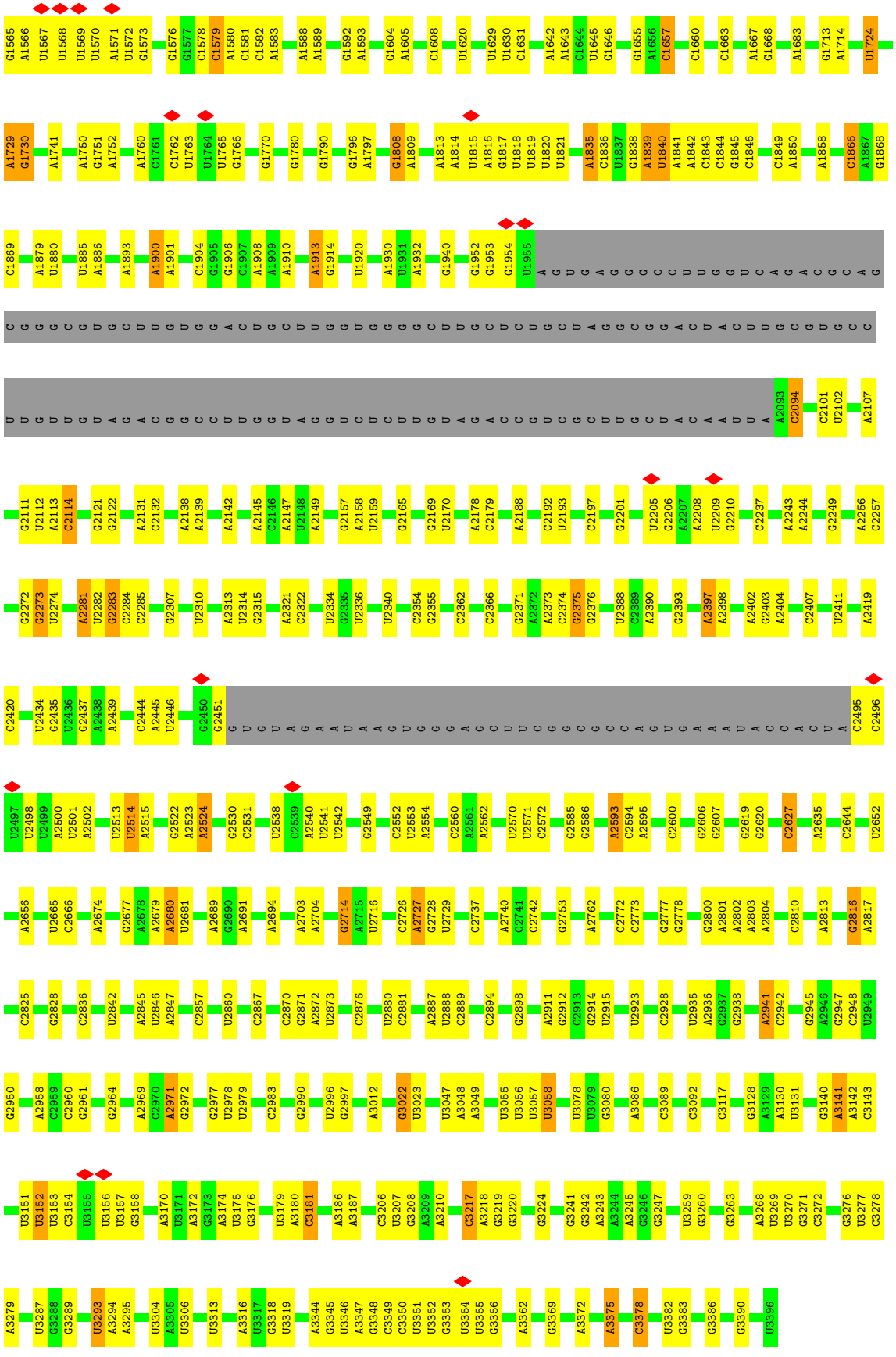




• Molecule 54: 25S ribosomal RNA

Chain BQ:



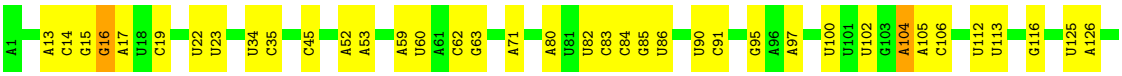


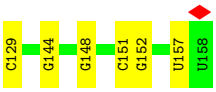
• Molecule 55: 5S ribosomal RNA

Chain BR:

• Molecule 56: 5.8S ribosomal RNA

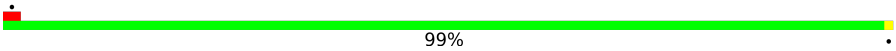
Chain BS:

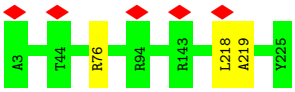




• Molecule 57: 40S ribosomal protein S3

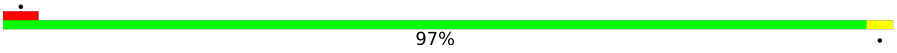
Chain A:

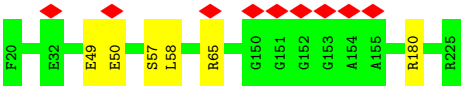




• Molecule 58: Rps5p

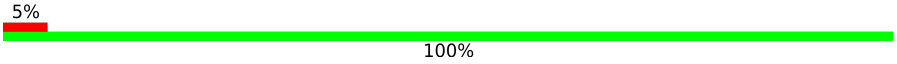
Chain B:

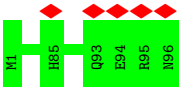




• Molecule 59: 40S ribosomal protein S10-A

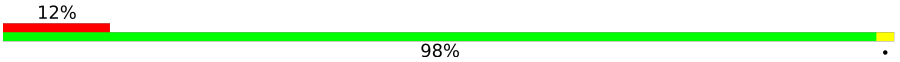
Chain C:

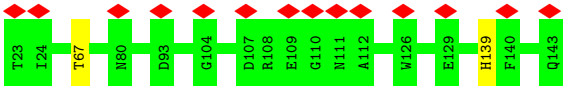




• Molecule 60: 40S ribosomal protein S12

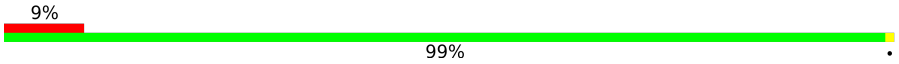
Chain D:

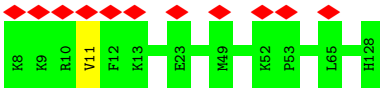




• Molecule 61: 40S ribosomal protein S15

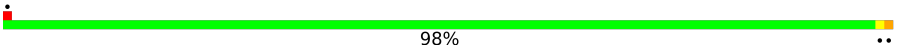
Chain E:

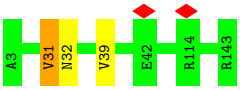




• Molecule 62: 40S ribosomal protein S16-A

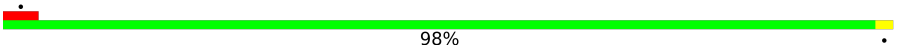
Chain F:

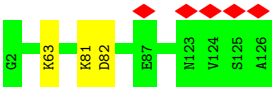




• Molecule 63: 40S ribosomal protein S17-A

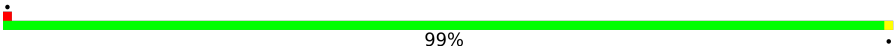
Chain G:

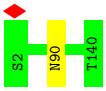




• Molecule 64: 40S ribosomal protein S18-A

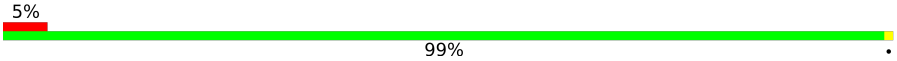
Chain H:

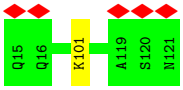




• Molecule 65: 40S ribosomal protein S20

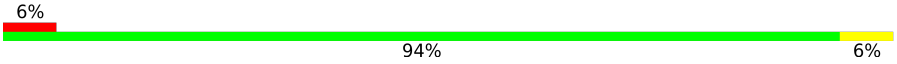
Chain J:

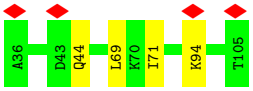




• Molecule 66: 40S ribosomal protein S25-A

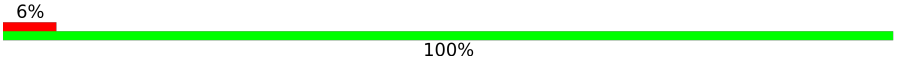
Chain K:

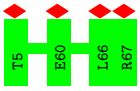




• Molecule 67: 40S ribosomal protein S28-A

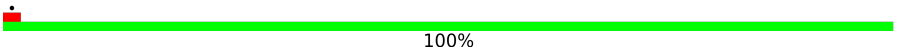
Chain L:





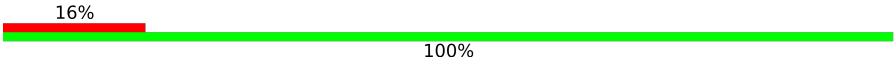
• Molecule 68: 40S ribosomal protein S29-A

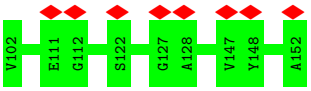
Chain M:



• Molecule 69: Ubiquitin-40S ribosomal protein S31

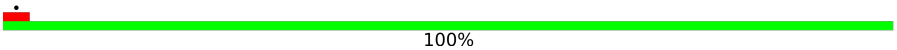
Chain N:

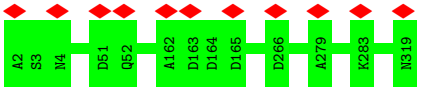




• Molecule 70: Guanine nucleotide-binding protein subunit beta-like protein

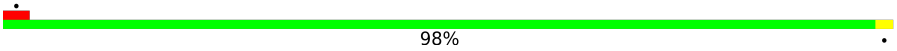
Chain O:





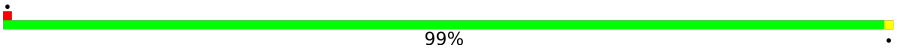
• Molecule 71: 40S ribosomal protein S0-A

Chain P:



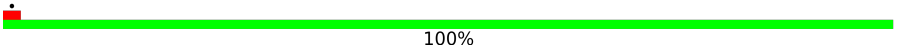
• Molecule 72: 40S ribosomal protein S1-A

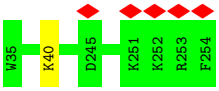
Chain Q:



• Molecule 73: 40S ribosomal protein S2

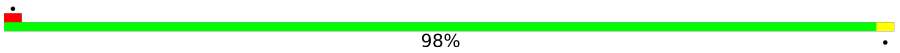
Chain R:

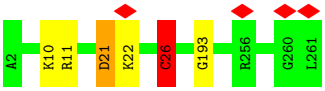




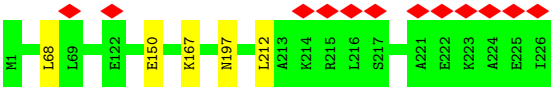
• Molecule 74: 40S ribosomal protein S4-A

Chain S:

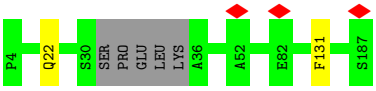




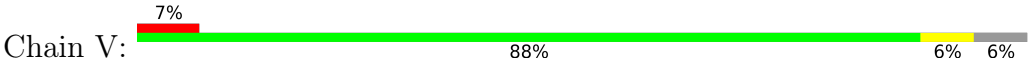
• Molecule 75: 40S ribosomal protein S6-A

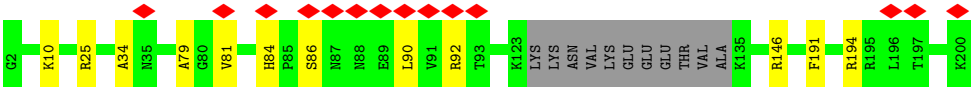


• Molecule 76: 40S ribosomal protein S7-A

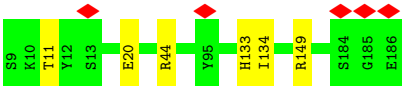


• Molecule 77: 40S ribosomal protein S8-A

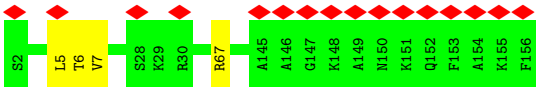




• Molecule 78: 40S ribosomal protein S9-A



• Molecule 79: 40S ribosomal protein S11-A



• Molecule 80: 40S ribosomal protein S13

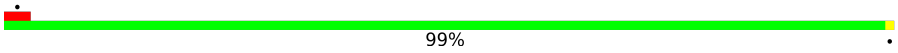
• Molecule 81: 40S ribosomal protein S14-B

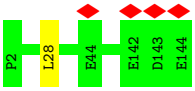
Chain Z:

There are no outlier residues recorded for this chain.

• Molecule 82: 40S ribosomal protein S19-A

Chain I:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217000	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 ($e^-/Å^2$)	2.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.470	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	433.6, 433.6, 433.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	2	1.09	8/42103 (0.0%)	1.12	119/65603 (0.2%)
2	AA	0.65	1/1836 (0.1%)	0.66	0/2481
3	AB	0.70	0/1018	0.75	2/1369 (0.1%)
4	AC	0.56	0/778	0.70	0/1034
5	AD	0.59	0/1539	0.68	0/2073
6	AE	0.72	0/555	0.67	0/738
7	AF	0.88	0/696	0.92	2/923 (0.2%)
8	AG	0.48	0/1374	0.66	0/1842
9	AH	0.72	0/979	0.70	0/1321
10	AI	0.57	0/618	0.64	0/826
11	AJ	0.73	0/1568	0.82	4/2106 (0.2%)
12	AK	0.68	0/1004	0.72	0/1341
13	AL	0.79	0/443	0.90	2/588 (0.3%)
14	AM	0.60	0/1068	0.73	1/1438 (0.1%)
15	AN	0.69	0/1118	0.63	0/1497
16	AO	0.58	0/423	0.73	0/562
17	AP	0.70	0/860	0.74	2/1136 (0.2%)
18	AQ	0.94	0/1757	0.92	9/2354 (0.4%)
19	AR	0.79	0/1204	0.79	3/1612 (0.2%)
20	AS	0.73	0/234	1.04	1/300 (0.3%)
21	AT	0.80	0/701	0.82	1/934 (0.1%)
22	AU	0.75	0/1585	0.70	2/2128 (0.1%)
23	AV	0.57	0/473	0.66	0/629
24	AW	0.84	1/1948 (0.1%)	0.87	11/2617 (0.4%)
25	AX	0.74	0/1443	0.79	4/1944 (0.2%)
26	a	0.60	0/693	0.69	0/935
27	b	0.71	0/1038	0.67	0/1395
28	c	0.66	0/1139	0.78	2/1518 (0.1%)
29	d	0.48	0/1074	0.71	0/1431
30	e	0.68	0/782	0.98	3/1047 (0.3%)
31	f	0.55	0/620	0.67	0/838
32	g	0.44	0/481	0.65	0/640

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	z	0.37	0/7362	0.69	6/9944 (0.1%)
34	l	0.69	0/411	0.95	0/639
35	n	0.76	0/1811	1.03	4/2821 (0.1%)
36	m	0.54	0/1773	0.99	2/2759 (0.1%)
37	AY	0.67	0/750	0.67	1/1008 (0.1%)
38	BA	0.77	1/3146 (0.0%)	0.75	3/4228 (0.1%)
39	BB	0.70	0/1465	0.80	3/1965 (0.2%)
40	BC	0.70	0/890	0.76	1/1196 (0.1%)
41	BD	0.62	0/1807	0.71	1/2425 (0.0%)
42	BE	0.74	1/2800 (0.0%)	0.73	2/3790 (0.1%)
43	BF	0.70	0/1538	0.79	4/2050 (0.2%)
44	BG	0.74	1/1041 (0.1%)	0.73	0/1394
45	BH	0.72	0/1481	0.70	0/1990
46	BI	0.56	0/2425	0.63	1/3271 (0.0%)
47	BJ	0.71	0/1300	0.73	2/1743 (0.1%)
48	BK	0.85	0/868	0.74	0/1168
49	BL	0.56	0/812	0.56	0/1099
50	BM	0.56	0/1260	0.65	1/1694 (0.1%)
51	BN	0.82	0/890	0.79	2/1189 (0.2%)
52	BO	0.74	0/1821	0.68	2/2451 (0.1%)
53	BP	0.65	0/978	0.78	5/1301 (0.4%)
54	BQ	1.43	82/75679 (0.1%)	1.24	287/117989 (0.2%)
55	BR	1.08	0/2883	1.03	2/4491 (0.0%)
56	BS	1.47	4/3745 (0.1%)	1.21	6/5829 (0.1%)
57	A	0.46	0/1759	0.60	1/2368 (0.0%)
58	B	0.43	0/1623	0.65	1/2195 (0.0%)
59	C	0.40	0/833	0.56	0/1126
60	D	0.35	0/885	0.65	0/1202
61	E	0.39	0/978	0.66	0/1315
62	F	0.52	0/1119	0.64	0/1503
63	G	0.45	0/1011	0.68	0/1355
64	H	0.39	0/1162	0.68	0/1564
65	J	0.44	0/865	0.61	0/1169
66	K	0.38	0/571	0.74	1/768 (0.1%)
67	L	0.46	0/499	0.72	0/670
68	M	0.54	0/452	0.64	0/600
69	N	0.32	0/404	0.64	0/542
70	O	0.35	0/2489	0.58	0/3389
71	P	0.52	0/1732	0.65	0/2371
72	Q	0.53	0/1735	0.71	0/2335
73	R	0.62	0/1702	0.68	0/2310
74	S	0.57	0/2102	0.68	2/2829 (0.1%)
75	T	0.44	0/1823	0.71	0/2439

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	U	0.46	0/1465	0.62	0/1971
77	V	0.63	1/1514 (0.1%)	0.81	3/2021 (0.1%)
78	W	0.53	0/1456	0.74	1/1949 (0.1%)
79	X	0.76	0/1239	0.70	1/1673 (0.1%)
80	Y	0.65	0/1215	0.77	2/1638 (0.1%)
81	Z	0.63	0/901	0.80	0/1217
82	I	0.46	0/1119	0.59	0/1504
All	All	1.07	100/224741 (0.0%)	1.03	515/329657 (0.2%)

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
2	AA	0	3
4	AC	0	2
5	AD	0	1
10	AI	0	1
11	AJ	0	1
18	AQ	0	1
19	AR	0	1
21	AT	0	1
26	a	0	1
27	b	0	1
29	d	0	3
30	e	0	7
33	z	0	5
40	BC	0	1
41	BD	0	3
42	BE	0	1
46	BI	0	1
52	BO	0	1
53	BP	0	2
57	A	0	1
58	B	0	2
61	E	0	1
64	H	0	1
66	K	0	1
71	P	0	2
72	Q	0	2
74	S	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
75	T	0	3
76	U	0	1
77	V	0	6
78	W	0	2
79	X	0	1
80	Y	0	1
All	All	0	62

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BQ	1835	A	N9-C4	-6.43	1.33	1.37
54	BQ	906	A	N9-C4	-6.40	1.34	1.37
54	BQ	42	C	C4-C5	-6.31	1.38	1.43
54	BQ	2145	A	C8-N7	-6.31	1.27	1.31
54	BQ	3344	A	N9-C4	-6.07	1.34	1.37
54	BQ	1524	A	N9-C4	-5.96	1.34	1.37
54	BQ	2321	A	N9-C4	-5.92	1.34	1.37
54	BQ	820	A	C6-N6	-5.90	1.29	1.33
54	BQ	914	A	N9-C4	-5.89	1.34	1.37
54	BQ	650	C	C5-C6	-5.85	1.29	1.34
54	BQ	94	G	C6-N1	-5.84	1.35	1.39
54	BQ	279	U	C2-N3	-5.83	1.33	1.37
54	BQ	2321	A	C6-N6	-5.82	1.29	1.33
54	BQ	657	A	C6-N6	-5.81	1.29	1.33
54	BQ	665	A	N9-C4	-5.78	1.34	1.37
54	BQ	2407	C	C4-C5	-5.74	1.38	1.43
54	BQ	361	A	N9-C4	-5.72	1.34	1.37
1	2	978	A	C6-N6	-5.71	1.29	1.33
54	BQ	1432	C	C4-N4	-5.70	1.28	1.33
54	BQ	1496	C	C4-C5	-5.68	1.38	1.43
54	BQ	34	A	N7-C5	-5.68	1.35	1.39
54	BQ	1433	A	N9-C4	-5.67	1.34	1.37
54	BQ	360	G	C6-N1	-5.67	1.35	1.39
54	BQ	906	A	C6-N6	-5.65	1.29	1.33
54	BQ	963	G	C8-N7	-5.65	1.27	1.30
54	BQ	929	A	N9-C4	-5.63	1.34	1.37
54	BQ	2876	C	C4-C5	-5.62	1.38	1.43
42	BE	52	VAL	CB-CG2	-5.60	1.41	1.52
54	BQ	2948	C	C4-C5	-5.59	1.38	1.43
54	BQ	647	A	N9-C4	-5.58	1.34	1.37
54	BQ	2828	G	N9-C8	-5.58	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BQ	1143	A	N9-C4	-5.57	1.34	1.37
54	BQ	1835	A	N7-C5	-5.51	1.35	1.39
54	BQ	2149	A	C6-N6	-5.50	1.29	1.33
54	BQ	2828	G	N7-C5	-5.50	1.35	1.39
54	BQ	409	A	C6-N6	-5.49	1.29	1.33
54	BQ	927	C	C4-C5	-5.47	1.38	1.43
54	BQ	1843	C	C5-C6	-5.47	1.29	1.34
54	BQ	2149	A	N9-C4	-5.46	1.34	1.37
54	BQ	656	A	N7-C5	-5.43	1.35	1.39
54	BQ	1835	A	C6-N1	-5.43	1.31	1.35
54	BQ	42	C	C5-C6	-5.42	1.30	1.34
54	BQ	63	A	C6-N6	-5.37	1.29	1.33
77	V	81	VAL	CB-CG1	5.37	1.64	1.52
38	BA	84	VAL	CB-CG1	-5.35	1.41	1.52
54	BQ	940	G	N7-C5	-5.34	1.36	1.39
2	AA	50	VAL	CB-CG2	-5.32	1.41	1.52
54	BQ	1842	A	N9-C4	-5.32	1.34	1.37
54	BQ	345	G	C6-N1	-5.30	1.35	1.39
1	2	1777	G	C8-N7	-5.30	1.27	1.30
54	BQ	937	G	C6-N1	-5.29	1.35	1.39
54	BQ	1843	C	C4-C5	-5.29	1.38	1.43
54	BQ	340	C	C4-N4	-5.27	1.29	1.33
54	BQ	2407	C	C5-C6	-5.26	1.30	1.34
54	BQ	2969	A	N7-C5	-5.25	1.36	1.39
54	BQ	900	G	C8-N7	-5.24	1.27	1.30
54	BQ	39	A	C6-N6	-5.22	1.29	1.33
54	BQ	98	G	C6-N1	-5.22	1.35	1.39
1	2	1351	G	O3'-P	-5.21	1.54	1.61
54	BQ	837	A	C6-N6	-5.21	1.29	1.33
56	BS	45	C	C4-C5	-5.20	1.38	1.43
56	BS	104	A	C6-N6	-5.18	1.29	1.33
54	BQ	2958	A	N9-C4	-5.17	1.34	1.37
54	BQ	803	C	C5-C6	-5.16	1.30	1.34
54	BQ	1869	C	C4-C5	-5.16	1.38	1.43
1	2	1091	A	N9-C4	-5.16	1.34	1.37
1	2	1633	A	C6-N1	-5.15	1.31	1.35
54	BQ	1836	C	C5-C6	-5.14	1.30	1.34
54	BQ	963	G	N7-C5	-5.14	1.36	1.39
44	BG	51	SER	C-N	-5.14	1.22	1.34
56	BS	14	C	C5-C6	-5.14	1.30	1.34
54	BQ	920	A	N9-C4	-5.13	1.34	1.37
54	BQ	268	A	N9-C4	-5.13	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	14	C	C4-C5	-5.13	1.38	1.43
56	BS	13	A	C6-N6	-5.12	1.29	1.33
54	BQ	1844	C	C5-C6	-5.12	1.30	1.34
54	BQ	2620	G	N9-C4	-5.11	1.33	1.38
54	BQ	913	A	C6-N6	-5.11	1.29	1.33
54	BQ	319	A	C6-N6	-5.10	1.29	1.33
54	BQ	2813	A	C6-N1	-5.09	1.31	1.35
1	2	1787	C	C4-C5	-5.09	1.38	1.43
54	BQ	1304	A	O3'-P	-5.09	1.55	1.61
54	BQ	2355	G	C8-N7	-5.09	1.27	1.30
54	BQ	349	A	C6-N6	-5.08	1.29	1.33
54	BQ	2132	C	C5-C6	-5.08	1.30	1.34
54	BQ	857	G	C2-N3	-5.07	1.28	1.32
54	BQ	2322	C	C4-C5	-5.07	1.38	1.43
54	BQ	1141	C	C4-C5	-5.07	1.38	1.43
54	BQ	920	A	C5-C6	-5.06	1.36	1.41
54	BQ	1608	C	C4-C5	-5.06	1.39	1.43
54	BQ	2157	G	C6-N1	-5.06	1.36	1.39
24	AW	207	VAL	CB-CG1	-5.05	1.42	1.52
54	BQ	1432	C	C5-C6	-5.05	1.30	1.34
1	2	1012	U	C2-N3	-5.04	1.34	1.37
54	BQ	361	A	C6-N6	-5.04	1.29	1.33
54	BQ	658	G	N7-C5	-5.03	1.36	1.39
54	BQ	340	C	C5-C6	-5.02	1.30	1.34
54	BQ	2390	A	C6-N6	-5.02	1.29	1.33
54	BQ	2354	C	C5-C6	-5.01	1.30	1.34
54	BQ	1529	A	N9-C4	-5.00	1.34	1.37

All (515) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BQ	3152	U	C2-N1-C1'	10.51	130.31	117.70
54	BQ	406	G	O4'-C1'-N9	9.53	115.82	108.20
54	BQ	1303	A	C1'-C2'-O2'	-9.52	82.04	110.60
54	BQ	895	A	N9-C4-C5	-9.39	102.04	105.80
54	BQ	3344	A	N1-C6-N6	9.33	124.20	118.60
1	2	50	C	C2-N1-C1'	9.14	128.85	118.80
35	n	75	C	N3-C2-O2	-9.06	115.55	121.90
24	AW	9	ARG	NE-CZ-NH1	-8.89	115.85	120.30
54	BQ	1144	U	N3-C4-O4	8.83	125.58	119.40
54	BQ	556	U	C5-C4-O4	-8.77	120.64	125.90
54	BQ	2828	G	N7-C8-N9	8.48	117.34	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BQ	895	A	N3-C4-N9	8.38	134.10	127.40
1	2	54	C	N3-C2-O2	-8.18	116.17	121.90
1	2	1458	G	C4-N9-C1'	8.09	137.01	126.50
1	2	1246	C	N1-C2-O2	8.02	123.71	118.90
54	BQ	1840	U	C2-N1-C1'	8.00	127.30	117.70
1	2	1465	C	C2'-C3'-O3'	7.91	126.90	109.50
54	BQ	556	U	N3-C4-O4	7.78	124.85	119.40
54	BQ	3344	A	C5-N7-C8	-7.76	100.02	103.90
36	m	38	C	C6-N1-C2	-7.74	117.20	120.30
54	BQ	1144	U	C5-C4-O4	-7.64	121.31	125.90
24	AW	3	ARG	NE-CZ-NH2	-7.58	116.51	120.30
54	BQ	1496	C	C6-N1-C2	-7.53	117.29	120.30
1	2	1791	A	N1-C6-N6	7.46	123.08	118.60
54	BQ	1483	G	C8-N9-C4	-7.39	103.44	106.40
25	AX	82	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	2	1246	C	N3-C2-O2	-7.37	116.75	121.90
1	2	1533	C	N1-C2-O2	7.35	123.31	118.90
1	2	1458	G	C8-N9-C1'	-7.34	117.46	127.00
1	2	1389	C	C2-N1-C1'	7.33	126.87	118.80
54	BQ	895	A	C4-C5-N7	7.32	114.36	110.70
1	2	1791	A	C5-C6-N6	-7.31	117.85	123.70
13	AL	42	ARG	NE-CZ-NH2	-7.26	116.67	120.30
25	AX	82	ARG	NE-CZ-NH2	-7.25	116.67	120.30
54	BQ	2857	C	N1-C2-O2	7.24	123.25	118.90
1	2	1145	U	C2-N1-C1'	7.23	126.38	117.70
1	2	54	C	N1-C2-O2	7.23	123.24	118.90
1	2	656	G	C4-N9-C1'	7.21	135.88	126.50
54	BQ	915	A	N7-C8-N9	7.21	117.41	113.80
54	BQ	656	A	N7-C8-N9	7.14	117.37	113.80
1	2	361	C	N1-C2-O2	7.12	123.17	118.90
30	e	10	ARG	NE-CZ-NH2	7.12	123.86	120.30
54	BQ	3152	U	C6-N1-C1'	-7.12	111.24	121.20
54	BQ	1432	C	N3-C4-C5	7.10	124.74	121.90
1	2	1533	C	N3-C2-O2	-7.09	116.94	121.90
33	z	188	LEU	CA-CB-CG	7.06	131.54	115.30
1	2	53	G	N3-C4-N9	7.06	130.23	126.00
1	2	1765	A	O4'-C1'-N9	7.05	113.84	108.20
18	AQ	162	ARG	NE-CZ-NH2	-7.04	116.78	120.30
54	BQ	1144	U	C6-N1-C2	-7.01	116.79	121.00
1	2	55	A	O4'-C1'-N9	7.01	113.81	108.20
1	2	50	C	C6-N1-C1'	-6.99	112.41	120.80
24	AW	3	ARG	NE-CZ-NH1	6.95	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1258	U	N3-C2-O2	-6.90	117.37	122.20
35	n	75	C	C6-N1-C2	-6.90	117.54	120.30
54	BQ	2407	C	N1-C2-O2	6.88	123.03	118.90
54	BQ	2094	C	N3-C2-O2	-6.82	117.13	121.90
18	AQ	162	ARG	NE-CZ-NH1	6.77	123.69	120.30
54	BQ	800	G	C4-N9-C1'	6.75	135.27	126.50
54	BQ	922	U	C2-N1-C1'	6.74	125.79	117.70
24	AW	200	ARG	NE-CZ-NH2	6.73	123.67	120.30
54	BQ	1447	G	P-O3'-C3'	6.73	127.78	119.70
1	2	1541	G	N3-C2-N2	-6.71	115.21	119.90
54	BQ	3152	U	N1-C2-O2	6.69	127.48	122.80
54	BQ	211	A	P-O3'-C3'	6.64	127.67	119.70
54	BQ	1496	C	C2-N1-C1'	6.64	126.11	118.80
54	BQ	3344	A	C4-C5-N7	6.63	114.02	110.70
54	BQ	1904	C	C5-C4-N4	-6.63	115.56	120.20
1	2	1480	G	C4-N9-C1'	6.62	135.10	126.50
54	BQ	3362	A	N1-C6-N6	6.62	122.57	118.60
54	BQ	1808	G	C8-N9-C4	-6.59	103.76	106.40
1	2	1363	U	N1-C2-O2	6.58	127.40	122.80
54	BQ	3362	A	C5-N7-C8	-6.57	100.61	103.90
1	2	1158	C	C6-N1-C2	-6.57	117.67	120.30
54	BQ	3141	A	N1-C6-N6	6.57	122.54	118.60
1	2	934	C	C2-N1-C1'	6.56	126.01	118.80
54	BQ	98	G	C2-N3-C4	-6.55	108.62	111.90
54	BQ	3344	A	C5-C6-N6	-6.54	118.46	123.70
1	2	1363	U	N3-C2-O2	-6.52	117.63	122.20
24	AW	227	ARG	NE-CZ-NH2	-6.52	117.04	120.30
38	BA	244	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BQ	42	C	N1-C2-O2	6.50	122.80	118.90
54	BQ	2407	C	C5-C6-N1	6.48	124.24	121.00
54	BQ	2237	C	N1-C2-O2	6.48	122.79	118.90
57	A	218	LEU	CA-CB-CG	6.48	130.20	115.30
54	BQ	895	A	C6-C5-N7	-6.48	127.77	132.30
1	2	50	C	C5-C4-N4	-6.47	115.67	120.20
33	z	342	LEU	CA-CB-CG	6.47	130.18	115.30
1	2	427	C	N1-C2-O2	6.46	122.78	118.90
1	2	1274	C	P-O3'-C3'	6.45	127.44	119.70
54	BQ	963	G	C6-C5-N7	-6.44	126.53	130.40
54	BQ	3217	C	C2-N1-C1'	6.40	125.84	118.80
54	BQ	3047	U	C2-N1-C1'	6.40	125.38	117.70
54	BQ	3152	U	N3-C2-O2	-6.39	117.72	122.20
54	BQ	2870	C	N3-C2-O2	-6.39	117.43	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AU	18	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	2	610	G	C4-N9-C1'	6.38	134.80	126.50
17	AP	41	ARG	NE-CZ-NH1	6.38	123.49	120.30
54	BQ	1144	U	C5-C6-N1	6.38	125.89	122.70
30	e	8	ASN	CB-CA-C	6.38	123.16	110.40
79	X	5	LEU	CA-CB-CG	6.38	129.97	115.30
54	BQ	1483	G	N7-C8-N9	6.38	116.29	113.10
37	AY	34	LEU	CA-CB-CG	6.36	129.92	115.30
33	z	339	LEU	CA-CB-CG	6.36	129.92	115.30
54	BQ	1657	C	N3-C2-O2	-6.35	117.45	121.90
1	2	978	A	C5-C6-N1	6.35	120.87	117.70
54	BQ	1657	C	N1-C2-O2	6.34	122.70	118.90
1	2	830	U	C5-C4-O4	-6.34	122.10	125.90
18	AQ	108	ARG	NE-CZ-NH1	6.33	123.46	120.30
54	BQ	800	G	C8-N9-C1'	-6.33	118.78	127.00
54	BQ	3022	G	P-O3'-C3'	6.31	127.27	119.70
54	BQ	1418	A	N7-C8-N9	6.29	116.94	113.80
54	BQ	659	G	C2-N3-C4	-6.29	108.76	111.90
54	BQ	1578	C	N3-C2-O2	-6.29	117.50	121.90
54	BQ	1858	A	O4'-C1'-N9	6.28	113.23	108.20
1	2	190	C	N3-C2-O2	-6.28	117.51	121.90
54	BQ	2193	U	N3-C2-O2	-6.27	117.81	122.20
54	BQ	648	C	C5-C4-N4	-6.25	115.82	120.20
54	BQ	2828	G	C4-N9-C1'	6.25	134.62	126.50
1	2	555	A	N1-C2-N3	6.24	132.42	129.30
51	BN	74	ARG	NE-CZ-NH2	-6.23	117.19	120.30
54	BQ	2273	G	P-O3'-C3'	6.23	127.17	119.70
1	2	1469	A	C2'-C3'-O3'	6.21	123.64	113.70
54	BQ	2281	A	O4'-C1'-N9	6.21	113.17	108.20
1	2	656	G	C8-N9-C1'	-6.18	118.97	127.00
54	BQ	1307	G	C2'-C3'-O3'	6.18	123.59	113.70
1	2	1291	G	N3-C4-N9	-6.17	122.30	126.00
54	BQ	1317	A	O4'-C1'-N9	6.17	113.14	108.20
54	BQ	963	G	C4-C5-N7	6.17	113.27	110.80
54	BQ	900	G	C2-N3-C4	-6.16	108.82	111.90
54	BQ	2876	C	C6-N1-C2	-6.16	117.84	120.30
53	BP	86	ARG	NE-CZ-NH2	-6.15	117.22	120.30
54	BQ	2285	C	C5-C4-N4	-6.14	115.90	120.20
54	BQ	2620	G	N3-C4-N9	-6.14	122.32	126.00
54	BQ	657	A	C5-C6-N6	-6.13	118.79	123.70
54	BQ	155	G	P-O3'-C3'	6.12	127.04	119.70
54	BQ	3048	A	O4'-C1'-N9	6.12	113.09	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	260	U	C6-N1-C2	-6.11	117.34	121.00
54	BQ	1277	C	N1-C2-O2	6.09	122.55	118.90
54	BQ	35	A	C5-C6-N6	-6.07	118.85	123.70
1	2	1773	C	C6-N1-C2	-6.06	117.88	120.30
55	BR	77	G	O4'-C1'-N9	6.05	113.04	108.20
1	2	1777	G	C4-C5-N7	6.04	113.22	110.80
54	BQ	3181	C	N1-C2-O2	6.04	122.52	118.90
7	AF	65	ARG	NE-CZ-NH2	-6.03	117.29	120.30
54	BQ	422	A	C5-C6-N6	-6.02	118.89	123.70
54	BQ	3306	U	N3-C2-O2	-6.01	117.99	122.20
54	BQ	1910	A	C5-N7-C8	-6.00	100.90	103.90
1	2	50	C	N1-C2-O2	6.00	122.50	118.90
54	BQ	2407	C	C6-N1-C2	-6.00	117.90	120.30
1	2	361	C	N3-C2-O2	-5.99	117.70	121.90
19	AR	4	ARG	NE-CZ-NH1	5.99	123.30	120.30
54	BQ	1558	A	P-O3'-C3'	5.99	126.89	119.70
54	BQ	1724	U	O4'-C1'-N1	5.99	112.99	108.20
53	BP	86	ARG	NE-CZ-NH1	5.98	123.29	120.30
54	BQ	2941	A	P-O3'-C3'	5.97	126.87	119.70
54	BQ	2870	C	N1-C2-O2	5.97	122.48	118.90
54	BQ	1808	G	N7-C8-N9	5.97	116.08	113.10
54	BQ	3278	C	C2-N1-C1'	5.95	125.35	118.80
54	BQ	1064	A	P-O3'-C3'	5.93	126.82	119.70
54	BQ	1796	G	N3-C4-N9	-5.93	122.44	126.00
1	2	976	G	C2-N3-C4	-5.93	108.93	111.90
54	BQ	3344	A	N7-C8-N9	5.93	116.77	113.80
36	m	38	C	O4'-C1'-N1	5.93	112.94	108.20
54	BQ	42	C	C5-C4-N4	-5.93	116.05	120.20
1	2	260	U	N3-C2-O2	-5.92	118.06	122.20
40	BC	72	ARG	NE-CZ-NH2	-5.92	117.34	120.30
54	BQ	2836	C	C2-N1-C1'	5.92	125.31	118.80
54	BQ	1333	C	N1-C2-O2	5.89	122.44	118.90
54	BQ	1481	A	C3'-C2'-C1'	5.89	106.21	101.50
54	BQ	650	C	N1-C2-O2	5.88	122.42	118.90
54	BQ	1838	G	C2-N3-C4	-5.87	108.96	111.90
54	BQ	2803	A	C5-C6-N6	-5.86	119.01	123.70
54	BQ	1200	A	O4'-C1'-N9	5.85	112.88	108.20
1	2	1258	U	N1-C2-O2	5.85	126.89	122.80
54	BQ	2816	G	N3-C2-N2	-5.84	115.81	119.90
54	BQ	2593	A	P-O3'-C3'	5.83	126.70	119.70
1	2	1571	C	C2-N1-C1'	5.78	125.16	118.80
54	BQ	360	G	N1-C2-N2	-5.78	111.00	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BQ	1364	C	N1-C2-O2	5.78	122.36	118.90
54	BQ	3141	A	C5-C6-N6	-5.77	119.08	123.70
1	2	1297	G	N3-C4-N9	-5.77	122.54	126.00
7	AF	56	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BQ	890	C	C6-N1-C2	-5.76	118.00	120.30
54	BQ	2192	C	C6-N1-C2	-5.76	118.00	120.30
54	BQ	2192	C	N1-C2-O2	5.76	122.35	118.90
54	BQ	269	G	P-O3'-C3'	5.74	126.59	119.70
54	BQ	2727	A	P-O3'-C3'	5.74	126.59	119.70
54	BQ	2145	A	N7-C8-N9	5.73	116.67	113.80
1	2	965	U	C2-N1-C1'	5.73	124.57	117.70
1	2	736	C	N3-C2-O2	-5.72	117.89	121.90
54	BQ	1866	C	C6-N1-C2	-5.72	118.01	120.30
54	BQ	1910	A	N1-C6-N6	5.72	122.03	118.60
54	BQ	2961	G	N7-C8-N9	5.72	115.96	113.10
54	BQ	269	G	C8-N9-C4	-5.71	104.11	106.40
54	BQ	2355	G	C4-C5-N7	5.71	113.09	110.80
24	AW	179	LEU	CA-CB-CG	5.71	128.44	115.30
1	2	322	G	P-O3'-C3'	5.71	126.55	119.70
54	BQ	3152	U	C5-C6-N1	5.71	125.56	122.70
1	2	864	U	N3-C2-O2	-5.71	118.21	122.20
24	AW	21	ARG	NE-CZ-NH1	5.70	123.15	120.30
47	BJ	18	ASP	CB-CG-OD1	5.70	123.43	118.30
54	BQ	1491	A	C4-C5-N7	5.69	113.55	110.70
54	BQ	691	A	C5-C6-N6	-5.69	119.15	123.70
54	BQ	2600	C	N1-C2-O2	5.68	122.31	118.90
1	2	1389	C	C6-N1-C1'	-5.68	113.98	120.80
54	BQ	35	A	N1-C6-N6	5.68	122.01	118.60
54	BQ	36	C	N3-C4-C5	5.68	124.17	121.90
54	BQ	360	G	N3-C2-N2	5.68	123.88	119.90
1	2	400	A	C8-N9-C4	-5.68	103.53	105.80
24	AW	227	ARG	NE-CZ-NH1	5.68	123.14	120.30
42	BE	107	ARG	NE-CZ-NH1	5.67	123.14	120.30
54	BQ	2876	C	C5-C6-N1	5.67	123.83	121.00
1	2	1273	G	P-O3'-C3'	5.66	126.50	119.70
1	2	1481	C	N3-C4-N4	-5.66	114.04	118.00
33	z	98	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	2	1481	C	C5-C4-N4	5.66	124.16	120.20
1	2	1291	G	N3-C4-C5	5.66	131.43	128.60
11	AJ	35	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BQ	2193	U	N1-C2-O2	5.65	126.75	122.80
54	BQ	1910	A	N7-C8-N9	5.65	116.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BQ	970	A	C4-C5-N7	5.64	113.52	110.70
54	BQ	2366	C	C6-N1-C2	-5.63	118.05	120.30
24	AW	190	ARG	NE-CZ-NH1	-5.62	117.49	120.30
54	BQ	3293	U	P-O3'-C3'	5.62	126.44	119.70
54	BQ	1283	C	N3-C2-O2	-5.62	117.97	121.90
1	2	830	U	N3-C4-O4	5.62	123.33	119.40
54	BQ	1730	G	P-O3'-C3'	5.62	126.44	119.70
54	BQ	938	C	N1-C2-O2	5.61	122.27	118.90
1	2	53	G	N3-C4-C5	-5.61	125.80	128.60
54	BQ	364	G	C2-N3-C4	-5.61	109.10	111.90
54	BQ	1808	G	P-O3'-C3'	5.61	126.43	119.70
54	BQ	906	A	C5-N7-C8	-5.60	101.10	103.90
54	BQ	2881	C	C5-C4-N4	-5.60	116.28	120.20
39	BB	176	ARG	NE-CZ-NH2	5.57	123.09	120.30
54	BQ	2627	C	C6-N1-C2	-5.57	118.07	120.30
1	2	959	U	C2-N1-C1'	5.57	124.38	117.70
24	AW	9	ARG	NE-CZ-NH2	5.56	123.08	120.30
54	BQ	1496	C	C5-C6-N1	5.56	123.78	121.00
54	BQ	2680	A	P-O3'-C3'	5.56	126.38	119.70
54	BQ	190	U	N3-C2-O2	-5.56	118.31	122.20
1	2	614	C	N1-C2-O2	5.56	122.24	118.90
1	2	610	G	C8-N9-C1'	-5.55	119.78	127.00
21	AT	23	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	2	1258	U	C6-N1-C2	-5.55	117.67	121.00
54	BQ	2514	U	P-O3'-C3'	5.54	126.35	119.70
54	BQ	2714	G	C4-C5-N7	5.54	113.02	110.80
1	2	864	U	N1-C2-O2	5.54	126.68	122.80
1	2	628	G	C2-N3-C4	-5.54	109.13	111.90
38	BA	334	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	2	1458	G	N3-C4-N9	5.54	129.32	126.00
1	2	555	A	C8-N9-C4	-5.54	103.59	105.80
1	2	1770	U	N3-C4-O4	5.54	123.27	119.40
54	BQ	1908	A	C4-C5-N7	5.54	113.47	110.70
54	BQ	915	A	C8-N9-C4	-5.53	103.59	105.80
54	BQ	2960	C	C6-N1-C2	-5.53	118.09	120.30
54	BQ	2165	G	C2-N3-C4	-5.52	109.14	111.90
54	BQ	2375	G	N3-C2-N2	-5.52	116.03	119.90
54	BQ	893	C	C5-C4-N4	-5.52	116.34	120.20
54	BQ	3362	A	C4-C5-N7	5.52	113.46	110.70
17	AP	42	ARG	NE-CZ-NH1	5.51	123.06	120.30
54	BQ	1940	G	C5-C6-O6	5.51	131.91	128.60
3	AB	48	ARG	NE-CZ-NH2	-5.51	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1533	C	C6-N1-C2	-5.51	118.10	120.30
54	BQ	1525	G	C4-N9-C1'	5.51	133.66	126.50
54	BQ	3057	U	O5'-P-OP2	-5.51	100.74	105.70
1	2	656	G	N3-C4-N9	5.50	129.30	126.00
3	AB	48	ARG	NE-CZ-NH1	5.50	123.05	120.30
56	BS	16	G	C2-N3-C4	-5.50	109.15	111.90
18	AQ	50	ARG	NE-CZ-NH1	5.50	123.05	120.30
25	AX	135	ARG	NE-CZ-NH1	5.50	123.05	120.30
54	BQ	2813	A	C5-N7-C8	-5.50	101.15	103.90
54	BQ	691	A	O4'-C1'-N9	5.50	112.60	108.20
54	BQ	1655	G	C2-N3-C4	-5.49	109.15	111.90
54	BQ	2595	A	C4-C5-N7	5.49	113.44	110.70
54	BQ	656	A	C5-N7-C8	-5.49	101.16	103.90
54	BQ	1491	A	N9-C4-C5	-5.49	103.61	105.80
54	BQ	1579	C	N3-C2-O2	-5.49	118.06	121.90
54	BQ	1469	C	N1-C2-O2	5.49	122.19	118.90
1	2	1461	C	N1-C2-O2	5.48	122.19	118.90
11	AJ	70	ARG	NE-CZ-NH1	5.48	123.04	120.30
54	BQ	1839	A	N7-C8-N9	5.48	116.54	113.80
54	BQ	3375	A	C4-N9-C1'	5.48	136.16	126.30
1	2	1012	U	N3-C4-O4	5.47	123.23	119.40
47	BJ	83	ARG	NE-CZ-NH2	-5.47	117.56	120.30
54	BQ	3058	U	C2-N1-C1'	5.47	124.26	117.70
1	2	1030	A	N1-C6-N6	-5.46	115.32	118.60
1	2	1541	G	N3-C4-N9	-5.46	122.72	126.00
1	2	555	A	N7-C8-N9	5.46	116.53	113.80
54	BQ	970	A	C5-N7-C8	-5.46	101.17	103.90
54	BQ	1546	A	C5-C6-N6	-5.46	119.33	123.70
54	BQ	1604	G	C4-N9-C1'	5.46	133.59	126.50
54	BQ	885	U	C5-C6-N1	5.45	125.43	122.70
54	BQ	916	G	P-O3'-C3'	5.45	126.24	119.70
54	BQ	950	G	C2-N3-C4	-5.45	109.17	111.90
54	BQ	1869	C	C5-C4-N4	-5.45	116.39	120.20
1	2	1527	C	C5-C4-N4	-5.45	116.39	120.20
54	BQ	890	C	N3-C2-O2	-5.44	118.09	121.90
1	2	1127	G	C2-N3-C4	-5.43	109.18	111.90
11	AJ	49	ARG	NE-CZ-NH2	5.43	123.02	120.30
18	AQ	172	ARG	NE-CZ-NH2	-5.43	117.58	120.30
54	BQ	2147	A	N7-C8-N9	5.43	116.52	113.80
11	AJ	36	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	2	53	G	N3-C2-N2	5.43	123.70	119.90
1	2	1458	G	C6-C5-N7	-5.43	127.14	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1571	C	N1-C2-O2	5.42	122.16	118.90
1	2	1246	C	C2-N1-C1'	5.42	124.76	118.80
54	BQ	1729	A	N7-C8-N9	5.41	116.51	113.80
1	2	1246	C	C6-N1-C2	-5.41	118.14	120.30
18	AQ	63	ARG	NE-CZ-NH1	5.41	123.00	120.30
54	BQ	2524	A	O4'-C1'-N9	5.41	112.53	108.20
54	BQ	3362	A	N7-C8-N9	5.41	116.50	113.80
24	AW	64	ARG	NE-CZ-NH1	5.40	123.00	120.30
54	BQ	657	A	C4-C5-N7	5.40	113.40	110.70
77	V	90	LEU	CA-CB-CG	5.40	127.73	115.30
54	BQ	2971	A	P-O3'-C3'	5.40	126.18	119.70
54	BQ	1418	A	C5-N7-C8	-5.39	101.20	103.90
54	BQ	1277	C	N3-C2-O2	-5.39	118.13	121.90
54	BQ	2873	U	C2-N1-C1'	5.39	124.17	117.70
54	BQ	1913	A	OP1-P-O3'	5.38	117.04	105.20
20	AS	17	ARG	NE-CZ-NH1	5.38	122.99	120.30
54	BQ	320	G	N3-C4-N9	-5.38	122.77	126.00
54	BQ	154	U	P-O3'-C3'	5.38	126.15	119.70
54	BQ	374	A	P-O3'-C3'	5.37	126.15	119.70
54	BQ	1910	A	C5-C6-N6	-5.37	119.41	123.70
54	BQ	2828	G	C5-N7-C8	-5.37	101.62	104.30
1	2	1480	G	C8-N9-C1'	-5.36	120.03	127.00
54	BQ	2145	A	C4-C5-N7	5.36	113.38	110.70
1	2	1420	C	C5-C4-N4	-5.36	116.45	120.20
1	2	1787	C	N1-C2-O2	5.36	122.11	118.90
54	BQ	2846	U	C2-N1-C1'	5.36	124.13	117.70
80	Y	121	ARG	NE-CZ-NH1	5.36	122.98	120.30
54	BQ	3306	U	N1-C2-O2	5.35	126.55	122.80
54	BQ	1145	G	C2-N3-C4	-5.35	109.23	111.90
55	BR	77	G	P-O3'-C3'	5.35	126.12	119.70
51	BN	74	ARG	NE-CZ-NH1	5.34	122.97	120.30
54	BQ	1578	C	N1-C2-O2	5.34	122.10	118.90
54	BQ	1663	C	N1-C2-O2	5.34	122.10	118.90
54	BQ	2828	G	C6-C5-N7	-5.33	127.20	130.40
1	2	323	A	N7-C8-N9	5.33	116.47	113.80
14	AM	117	ARG	NE-CZ-NH1	5.33	122.97	120.30
54	BQ	1790	G	C2-N3-C4	-5.33	109.23	111.90
54	BQ	1657	C	N3-C4-N4	-5.33	114.27	118.00
54	BQ	1283	C	N1-C2-O2	5.33	122.10	118.90
54	BQ	3378	C	N1-C2-O2	5.33	122.10	118.90
1	2	50	C	N3-C4-N4	5.33	121.73	118.00
56	BS	15	G	C2-N3-C4	-5.33	109.24	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BQ	2873	U	N3-C2-O2	-5.32	118.48	122.20
54	BQ	2362	C	N1-C2-O2	5.32	122.09	118.90
78	W	44	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	2	868	G	N3-C4-N9	-5.31	122.81	126.00
54	BQ	340	C	N1-C2-O2	5.31	122.09	118.90
1	2	1571	C	N3-C2-O2	-5.30	118.19	121.90
52	BO	151	ARG	NE-CZ-NH1	5.30	122.95	120.30
42	BE	95	ARG	NE-CZ-NH2	-5.30	117.65	120.30
54	BQ	657	A	C5-C6-N1	5.30	120.35	117.70
54	BQ	3372	A	N7-C8-N9	5.29	116.45	113.80
1	2	105	A	O4'-C1'-N9	5.29	112.43	108.20
54	BQ	2397	A	N9-C4-C5	-5.29	103.68	105.80
39	BB	180	ARG	NE-CZ-NH1	5.29	122.95	120.30
54	BQ	2371	G	C2-N3-C4	-5.29	109.25	111.90
54	BQ	3089	C	N1-C2-O2	5.29	122.07	118.90
1	2	1672	G	C4-N9-C1'	5.29	133.38	126.50
50	BM	26	ARG	NE-CZ-NH1	5.29	122.94	120.30
54	BQ	1667	A	N7-C8-N9	5.29	116.44	113.80
54	BQ	968	G	N7-C8-N9	5.29	115.74	113.10
54	BQ	970	A	N9-C4-C5	-5.28	103.69	105.80
54	BQ	1900	A	C8-N9-C4	-5.28	103.69	105.80
54	BQ	1908	A	N9-C4-C5	-5.28	103.69	105.80
74	S	26	CYS	N-CA-C	5.28	125.25	111.00
1	2	765	G	OP1-P-O3'	5.27	116.80	105.20
54	BQ	915	A	C5-N7-C8	-5.27	101.26	103.90
54	BQ	771	A	N1-C6-N6	5.26	121.76	118.60
56	BS	100	U	C5-C6-N1	5.26	125.33	122.70
54	BQ	2876	C	C2-N1-C1'	5.26	124.59	118.80
1	2	54	C	C6-N1-C2	-5.26	118.20	120.30
54	BQ	2145	A	C5-N7-C8	-5.26	101.27	103.90
1	2	419	G	C2-N3-C4	-5.25	109.27	111.90
1	2	1182	U	C2-N1-C1'	5.25	124.00	117.70
54	BQ	2961	G	C8-N9-C4	-5.25	104.30	106.40
66	K	69	LEU	CA-CB-CG	5.25	127.38	115.30
54	BQ	3181	C	C2-N1-C1'	5.25	124.57	118.80
1	2	313	U	P-O3'-C3'	5.25	126.00	119.70
38	BA	334	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	2	400	A	N7-C8-N9	5.25	116.42	113.80
54	BQ	1729	A	N1-C6-N6	5.24	121.75	118.60
54	BQ	2514	U	OP1-P-O3'	5.24	116.73	105.20
54	BQ	3362	A	C5-C6-N6	-5.24	119.51	123.70
54	BQ	1194	G	N1-C6-O6	5.24	123.04	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BP	89	ARG	NE-CZ-NH1	5.24	122.92	120.30
54	BQ	2620	G	C2-N3-C4	-5.24	109.28	111.90
54	BQ	340	C	N3-C4-C5	5.23	123.99	121.90
54	BQ	657	A	C5-N7-C8	-5.23	101.28	103.90
54	BQ	895	A	C8-N9-C1'	-5.23	118.28	127.70
54	BQ	1869	C	N3-C4-C5	5.23	123.99	121.90
28	c	13	ARG	NE-CZ-NH1	5.23	122.92	120.30
54	BQ	2142	A	C5-C6-N6	-5.23	119.52	123.70
33	z	652	LEU	CA-CB-CG	5.22	127.31	115.30
54	BQ	1120	A	C4-C5-N7	5.22	113.31	110.70
54	BQ	2950	G	O4'-C1'-N9	5.22	112.38	108.20
54	BQ	2964	G	N3-C4-N9	-5.22	122.87	126.00
54	BQ	58	G	C5-C6-O6	5.21	131.73	128.60
18	AQ	108	ARG	NE-CZ-NH2	-5.21	117.69	120.30
56	BS	45	C	N1-C2-O2	5.21	122.03	118.90
80	Y	28	LEU	CA-CB-CG	5.21	127.28	115.30
1	2	429	G	C2-N3-C4	5.21	114.50	111.90
1	2	453	U	C6-N1-C2	-5.21	117.88	121.00
54	BQ	422	A	N1-C6-N6	5.21	121.72	118.60
54	BQ	2773	C	C6-N1-C2	-5.20	118.22	120.30
77	V	25	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	2	1573	A	P-O3'-C3'	5.19	125.93	119.70
1	2	1745	G	C2-N3-C4	-5.19	109.30	111.90
35	n	34	A	C5-C6-N6	-5.19	119.55	123.70
54	BQ	1910	A	C4-C5-N7	5.19	113.30	110.70
54	BQ	2283	G	P-O3'-C3'	5.19	125.93	119.70
56	BS	19	C	N1-C2-O2	5.19	122.01	118.90
1	2	1791	A	C4-C5-N7	5.18	113.29	110.70
54	BQ	42	C	N3-C4-N4	5.18	121.63	118.00
54	BQ	1483	G	N1-C2-N2	-5.18	111.54	116.20
54	BQ	1118	C	C6-N1-C2	-5.18	118.23	120.30
1	2	765	G	P-O3'-C3'	5.17	125.91	119.70
1	2	429	G	N3-C4-C5	-5.17	126.02	128.60
54	BQ	8	C	N1-C2-O2	5.17	122.00	118.90
54	BQ	543	C	N1-C2-O2	5.17	122.00	118.90
39	BB	38	ARG	NE-CZ-NH1	5.16	122.88	120.30
54	BQ	2726	C	N3-C2-O2	-5.16	118.29	121.90
54	BQ	927	C	C6-N1-C2	-5.16	118.24	120.30
1	2	1169	G	C2-N3-C4	-5.15	109.33	111.90
43	BF	100	ARG	NE-CZ-NH2	-5.15	117.72	120.30
53	BP	48	ARG	NE-CZ-NH1	5.15	122.88	120.30
54	BQ	33	G	C2-N3-C4	-5.15	109.33	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	656	G	N3-C4-C5	-5.15	126.03	128.60
46	BI	24	ARG	NE-CZ-NH1	5.15	122.87	120.30
19	AR	42	ARG	NE-CZ-NH1	5.14	122.87	120.30
19	AR	42	ARG	NE-CZ-NH2	-5.14	117.73	120.30
25	AX	23	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	2	1770	U	C5-C4-O4	-5.13	122.82	125.90
54	BQ	2813	A	C4-C5-N7	5.13	113.27	110.70
54	BQ	1189	C	C5-C4-N4	-5.13	116.61	120.20
1	2	1145	U	C6-N1-C1'	-5.13	114.02	121.20
1	2	964	U	C5-C6-N1	5.13	125.26	122.70
54	BQ	2828	G	C8-N9-C4	-5.13	104.35	106.40
54	BQ	1835	A	C5-N7-C8	-5.12	101.34	103.90
54	BQ	1424	C	C5-C4-N4	-5.12	116.61	120.20
54	BQ	1448	U	C5-C6-N1	5.12	125.26	122.70
1	2	1361	U	N1-C2-O2	5.12	126.38	122.80
41	BD	97	ARG	NE-CZ-NH1	5.12	122.86	120.30
54	BQ	21	G	C8-N9-C4	-5.11	104.35	106.40
54	BQ	288	C	C5-C4-N4	-5.11	116.62	120.20
54	BQ	638	C	N1-C2-O2	5.11	121.97	118.90
54	BQ	909	G	C2-N3-C4	-5.11	109.35	111.90
54	BQ	1496	C	N3-C4-N4	5.11	121.57	118.00
54	BQ	2825	C	C5-C4-N4	-5.11	116.63	120.20
1	2	1791	A	N9-C4-C5	-5.10	103.76	105.80
54	BQ	1667	A	C5-N7-C8	-5.10	101.35	103.90
1	2	1258	U	C5-C6-N1	5.10	125.25	122.70
1	2	1461	C	N3-C2-O2	-5.10	118.33	121.90
54	BQ	3293	U	OP1-P-O3'	5.10	116.41	105.20
54	BQ	857	G	C2-N3-C4	-5.10	109.35	111.90
52	BO	160	ARG	NE-CZ-NH1	5.09	122.85	120.30
54	BQ	1417	G	P-O3'-C3'	5.09	125.81	119.70
54	BQ	1496	C	N1-C2-O2	5.09	121.96	118.90
54	BQ	2355	G	C6-C5-N7	-5.09	127.34	130.40
54	BQ	2644	C	N1-C2-O2	5.09	121.95	118.90
54	BQ	920	A	C4-C5-N7	5.09	113.24	110.70
74	S	193	GLY	N-CA-C	5.08	125.81	113.10
54	BQ	2390	A	C5-N7-C8	-5.08	101.36	103.90
1	2	1592	A	N7-C8-N9	5.08	116.34	113.80
1	2	1773	C	C5-C6-N1	5.08	123.54	121.00
54	BQ	2273	G	C8-N9-C4	-5.08	104.37	106.40
54	BQ	3378	C	C6-N1-C2	-5.08	118.27	120.30
54	BQ	1437	C	C6-N1-C2	-5.08	118.27	120.30
43	BF	151	ARG	NE-CZ-NH1	5.07	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BQ	543	C	N3-C2-O2	-5.07	118.35	121.90
54	BQ	1448	U	C2-N1-C1'	5.07	123.78	117.70
54	BQ	1808	G	N1-C2-N2	-5.07	111.64	116.20
1	2	1112	G	C2-N3-C4	-5.06	109.37	111.90
54	BQ	1592	G	C2-N3-C4	-5.06	109.37	111.90
54	BQ	2880	U	C5-C6-N1	5.06	125.23	122.70
54	BQ	1840	U	C6-N1-C2	-5.06	117.97	121.00
54	BQ	2390	A	C4-C5-N7	5.06	113.23	110.70
30	e	61	GLU	C-N-CA	5.05	134.34	121.70
58	B	180	ARG	NE-CZ-NH1	5.05	122.83	120.30
54	BQ	906	A	C4-C5-C6	-5.05	114.47	117.00
13	AL	41	ARG	NE-CZ-NH1	5.05	122.83	120.30
56	BS	45	C	C2-N1-C1'	5.05	124.35	118.80
54	BQ	938	C	N3-C4-N4	5.04	121.53	118.00
1	2	1003	A	O4'-C1'-N9	5.04	112.23	108.20
54	BQ	2407	C	C2-N1-C1'	5.04	124.34	118.80
54	BQ	3344	A	C6-C5-N7	-5.04	128.77	132.30
54	BQ	651	G	N7-C8-N9	5.04	115.62	113.10
28	c	144	ARG	NE-CZ-NH2	5.03	122.82	120.30
54	BQ	818	C	N3-C4-C5	5.03	123.91	121.90
54	BQ	1660	C	N1-C2-O2	5.03	121.92	118.90
43	BF	103	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	2	928	U	P-O3'-C3'	5.03	125.73	119.70
54	BQ	2114	C	C6-N1-C2	-5.03	118.29	120.30
54	BQ	1303	A	N9-C1'-C2'	5.02	120.53	114.00
22	AU	101	ARG	NE-CZ-NH1	5.02	122.81	120.30
54	BQ	1668	G	N7-C8-N9	5.02	115.61	113.10
77	V	146	ARG	NE-CZ-NH1	5.02	122.81	120.30
54	BQ	1194	G	C4-C5-N7	5.01	112.81	110.80
54	BQ	2420	C	N1-C2-O2	5.01	121.91	118.90
35	n	34	A	N1-C6-N6	5.01	121.61	118.60
54	BQ	895	A	C5-C6-N1	5.01	120.21	117.70
54	BQ	1142	G	C2-N3-C4	-5.01	109.39	111.90
54	BQ	1796	G	C8-N9-C1'	5.01	133.51	127.00
18	AQ	144	ARG	NE-CZ-NH1	5.01	122.80	120.30
18	AQ	188	ARG	NE-CZ-NH1	5.01	122.80	120.30
54	BQ	1840	U	N1-C2-O2	5.00	126.30	122.80
54	BQ	2192	C	C2-N1-C1'	5.00	124.31	118.80
43	BF	85	ARG	NE-CZ-NH1	5.00	122.80	120.30
53	BP	38	ARG	NE-CZ-NH1	5.00	122.80	120.30
33	z	455	LEU	CA-CB-CG	5.00	126.80	115.30
54	BQ	359	U	C5-C6-N1	5.00	125.20	122.70

There are no chirality outliers.

All (62) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
57	A	219	ALA	Peptide
2	AA	156	ASP	Peptide
2	AA	74	THR	Peptide
2	AA	76	ALA	Peptide
4	AC	26	ILE	Peptide
4	AC	32	ALA	Peptide
5	AD	22	SER	Peptide
10	AI	34	ALA	Peptide
11	AJ	74	GLY	Peptide
18	AQ	92	LEU	Peptide
19	AR	2	PRO	Peptide
21	AT	49	ARG	Peptide
58	B	57	SER	Peptide
58	B	65	ARG	Peptide
40	BC	6	ASP	Peptide
41	BD	109	ARG	Peptide
41	BD	170	TRP	Peptide
41	BD	171	GLY	Peptide
42	BE	318	LEU	Peptide
46	BI	258	LYS	Peptide
52	BO	232	ARG	Peptide
53	BP	83	LYS	Peptide
53	BP	91	ALA	Peptide
61	E	11	VAL	Peptide
64	H	90	ASN	Peptide
66	K	44	GLN	Peptide
71	P	110	TYR	Peptide
71	P	157	ASP	Peptide
72	Q	152	ARG	Peptide
72	Q	223	PHE	Peptide
74	S	22	LYS	Peptide
75	T	150	GLU	Peptide
75	T	197	ASN	Peptide
75	T	212	LEU	Peptide
76	U	131	PHE	Peptide
77	V	191	PHE	Peptide
77	V	34	ALA	Peptide
77	V	79	ALA	Peptide
77	V	84	HIS	Peptide
77	V	86	SER	Peptide

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Mol	Chain	Res	Type	Group
77	V	92	ARG	Peptide
78	W	11	THR	Peptide
78	W	133	HIS	Peptide
79	X	6	THR	Peptide
80	Y	150	VAL	Peptide
26	a	81	ASN	Peptide
27	b	54	ASP	Peptide
29	d	119	PHE	Peptide
29	d	51	GLU	Peptide
29	d	52	LYS	Peptide
30	e	10	ARG	Peptide
30	e	15	ARG	Peptide
30	e	34	LYS	Peptide
30	e	61	GLU	Peptide
30	e	62	TYR	Peptide
30	e	7	SER	Peptide
30	e	84	VAL	Peptide
33	z	20	LEU	Peptide
33	z	267	GLU	Peptide
33	z	427	LYS	Peptide
33	z	675	LYS	Peptide
33	z	885	ILE	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
2	AA	231/233 (99%)	204 (88%)	25 (11%)	2 (1%)	17 52
3	AB	134/136 (98%)	129 (96%)	5 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	AC	97/100 (97%)	90 (93%)	5 (5%)	2 (2%)	7 30
5	AD	189/191 (99%)	175 (93%)	13 (7%)	1 (0%)	29 64
6	AE	65/67 (97%)	61 (94%)	4 (6%)	0	100 100
7	AF	85/87 (98%)	77 (91%)	8 (9%)	0	100 100
8	AG	167/169 (99%)	154 (92%)	12 (7%)	1 (1%)	25 59
9	AH	119/121 (98%)	115 (97%)	4 (3%)	0	100 100
10	AI	75/77 (97%)	69 (92%)	6 (8%)	0	100 100
11	AJ	191/193 (99%)	168 (88%)	19 (10%)	4 (2%)	7 30
12	AK	124/126 (98%)	123 (99%)	1 (1%)	0	100 100
13	AL	48/50 (96%)	45 (94%)	3 (6%)	0	100 100
14	AM	134/136 (98%)	121 (90%)	13 (10%)	0	100 100
15	AN	133/135 (98%)	117 (88%)	16 (12%)	0	100 100
16	AO	50/52 (96%)	47 (94%)	3 (6%)	0	100 100
17	AP	103/105 (98%)	92 (89%)	11 (11%)	0	100 100
18	AQ	201/203 (99%)	184 (92%)	16 (8%)	1 (0%)	29 64
19	AR	146/148 (99%)	125 (86%)	19 (13%)	2 (1%)	11 40
20	AS	23/25 (92%)	23 (100%)	0	0	100 100
21	AT	89/91 (98%)	81 (91%)	8 (9%)	0	100 100
22	AU	195/197 (99%)	188 (96%)	7 (4%)	0	100 100
23	AV	56/58 (97%)	53 (95%)	3 (5%)	0	100 100
24	AW	250/252 (99%)	238 (95%)	12 (5%)	0	100 100
25	AX	181/183 (99%)	174 (96%)	7 (4%)	0	100 100
26	a	85/87 (98%)	70 (82%)	13 (15%)	2 (2%)	6 27
27	b	127/129 (98%)	123 (97%)	4 (3%)	0	100 100
28	c	142/144 (99%)	125 (88%)	16 (11%)	1 (1%)	22 57
29	d	130/132 (98%)	112 (86%)	16 (12%)	2 (2%)	10 39
30	e	95/97 (98%)	73 (77%)	21 (22%)	1 (1%)	14 46
31	f	79/81 (98%)	69 (87%)	10 (13%)	0	100 100
32	g	58/60 (97%)	49 (84%)	9 (16%)	0	100 100
33	z	864/916 (94%)	783 (91%)	80 (9%)	1 (0%)	51 83
37	AY	95/97 (98%)	94 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BA	384/386 (100%)	354 (92%)	30 (8%)	0	100	100
39	BB	183/185 (99%)	169 (92%)	14 (8%)	0	100	100
40	BC	107/109 (98%)	97 (91%)	9 (8%)	1 (1%)	17	52
41	BD	218/220 (99%)	198 (91%)	19 (9%)	1 (0%)	29	64
42	BE	359/361 (99%)	322 (90%)	35 (10%)	2 (1%)	25	59
43	BF	186/188 (99%)	173 (93%)	12 (6%)	1 (0%)	29	64
44	BG	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
45	BH	170/172 (99%)	159 (94%)	11 (6%)	0	100	100
46	BI	294/296 (99%)	271 (92%)	22 (8%)	1 (0%)	41	73
47	BJ	157/159 (99%)	140 (89%)	15 (10%)	2 (1%)	12	42
48	BK	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
49	BL	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
50	BM	152/175 (87%)	144 (95%)	8 (5%)	0	100	100
51	BN	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
52	BO	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	29	64
53	BP	117/119 (98%)	110 (94%)	5 (4%)	2 (2%)	9	36
57	A	221/223 (99%)	205 (93%)	16 (7%)	0	100	100
58	B	204/206 (99%)	167 (82%)	34 (17%)	3 (2%)	10	39
59	C	94/96 (98%)	79 (84%)	15 (16%)	0	100	100
60	D	119/121 (98%)	81 (68%)	37 (31%)	1 (1%)	19	54
61	E	119/121 (98%)	98 (82%)	21 (18%)	0	100	100
62	F	139/141 (99%)	120 (86%)	16 (12%)	3 (2%)	6	29
63	G	123/125 (98%)	103 (84%)	18 (15%)	2 (2%)	9	37
64	H	137/139 (99%)	117 (85%)	20 (15%)	0	100	100
65	J	105/107 (98%)	94 (90%)	11 (10%)	0	100	100
66	K	68/70 (97%)	56 (82%)	11 (16%)	1 (2%)	10	39
67	L	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
68	M	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
69	N	49/51 (96%)	38 (78%)	11 (22%)	0	100	100
70	O	316/318 (99%)	294 (93%)	22 (7%)	0	100	100
71	P	217/219 (99%)	191 (88%)	23 (11%)	3 (1%)	11	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	Q	212/214 (99%)	179 (84%)	32 (15%)	1 (0%)	29	64
73	R	218/220 (99%)	196 (90%)	21 (10%)	1 (0%)	29	64
74	S	258/260 (99%)	225 (87%)	31 (12%)	2 (1%)	19	54
75	T	224/226 (99%)	199 (89%)	24 (11%)	1 (0%)	34	69
76	U	175/184 (95%)	160 (91%)	15 (9%)	0	100	100
77	V	184/199 (92%)	158 (86%)	25 (14%)	1 (0%)	29	64
78	W	176/178 (99%)	144 (82%)	30 (17%)	2 (1%)	14	46
79	X	153/155 (99%)	140 (92%)	12 (8%)	1 (1%)	22	57
80	Y	148/150 (99%)	138 (93%)	10 (7%)	0	100	100
81	Z	125/127 (98%)	112 (90%)	13 (10%)	0	100	100
82	I	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	22	57
All	All	11782/12024 (98%)	10635 (90%)	1093 (9%)	54 (0%)	32	64

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AA	156	ASP
2	AA	157	VAL
11	AJ	62	THR
42	BE	339	LEU
53	BP	91	ALA
58	B	50	GLU
58	B	58	LEU
63	G	82	ASP
71	P	110	TYR
71	P	111	ILE
11	AJ	77	LEU
26	a	81	ASN
29	d	35	VAL
30	e	63	ALA
62	F	32	ASN
73	R	40	LYS
74	S	21	ASP
74	S	26	CYS
78	W	134	ILE
4	AC	33	ALA
11	AJ	61	PRO
19	AR	47	LYS

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Mol	Chain	Res	Type
26	a	45	ALA
42	BE	292	SER
47	BJ	125	ALA
53	BP	90	ARG
62	F	31	VAL
72	Q	158	SER
5	AD	23	ARG
11	AJ	76	THR
19	AR	4	ARG
41	BD	138	ARG
46	BI	259	LYS
58	B	49	GLU
71	P	196	SER
77	V	10	LYS
4	AC	34	SER
8	AG	172	LEU
18	AQ	94	TYR
28	c	90	ASP
29	d	52	LYS
33	z	601	LYS
40	BC	7	VAL
47	BJ	18	ASP
52	BO	164	SER
60	D	67	THR
63	G	81	LYS
66	K	71	ILE
75	T	68	LEU
78	W	20	GLU
82	I	28	LEU
43	BF	131	ALA
62	F	39	VAL
79	X	7	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AA	187/191 (98%)	186 (100%)	1 (0%)	88 94
3	AB	104/104 (100%)	104 (100%)	0	100 100
4	AC	81/82 (99%)	80 (99%)	1 (1%)	71 88
5	AD	171/171 (100%)	171 (100%)	0	100 100
6	AE	56/59 (95%)	56 (100%)	0	100 100
7	AF	70/70 (100%)	70 (100%)	0	100 100
8	AG	147/147 (100%)	147 (100%)	0	100 100
9	AH	104/105 (99%)	104 (100%)	0	100 100
10	AI	68/68 (100%)	68 (100%)	0	100 100
11	AJ	154/154 (100%)	153 (99%)	1 (1%)	86 94
12	AK	109/109 (100%)	108 (99%)	1 (1%)	78 91
13	AL	45/45 (100%)	45 (100%)	0	100 100
14	AM	107/107 (100%)	107 (100%)	0	100 100
15	AN	115/115 (100%)	114 (99%)	1 (1%)	78 91
16	AO	47/47 (100%)	47 (100%)	0	100 100
17	AP	90/90 (100%)	90 (100%)	0	100 100
18	AQ	175/175 (100%)	174 (99%)	1 (1%)	86 94
19	AR	118/118 (100%)	117 (99%)	1 (1%)	81 92
20	AS	23/23 (100%)	23 (100%)	0	100 100
21	AT	71/71 (100%)	70 (99%)	1 (1%)	67 86
22	AU	160/160 (100%)	160 (100%)	0	100 100
23	AV	46/46 (100%)	46 (100%)	0	100 100
24	AW	193/194 (100%)	192 (100%)	1 (0%)	88 94
25	AX	140/145 (97%)	140 (100%)	0	100 100
26	a	74/74 (100%)	74 (100%)	0	100 100
27	b	110/110 (100%)	110 (100%)	0	100 100
28	c	119/119 (100%)	118 (99%)	1 (1%)	81 92
29	d	111/111 (100%)	111 (100%)	0	100 100
30	e	83/83 (100%)	82 (99%)	1 (1%)	71 88
31	f	70/70 (100%)	70 (100%)	0	100 100
32	g	50/51 (98%)	50 (100%)	0	100 100
33	z	783/842 (93%)	766 (98%)	17 (2%)	52 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	AY	81/81 (100%)	81 (100%)	0	100	100
38	BA	320/322 (99%)	317 (99%)	3 (1%)	78	91
39	BB	150/150 (100%)	150 (100%)	0	100	100
40	BC	92/96 (96%)	92 (100%)	0	100	100
41	BD	184/186 (99%)	184 (100%)	0	100	100
42	BE	288/288 (100%)	288 (100%)	0	100	100
43	BF	153/153 (100%)	153 (100%)	0	100	100
44	BG	109/109 (100%)	109 (100%)	0	100	100
45	BH	156/156 (100%)	156 (100%)	0	100	100
46	BI	244/244 (100%)	243 (100%)	1 (0%)	91	96
47	BJ	136/136 (100%)	135 (99%)	1 (1%)	84	93
48	BK	90/90 (100%)	90 (100%)	0	100	100
49	BL	87/87 (100%)	87 (100%)	0	100	100
50	BM	134/152 (88%)	133 (99%)	1 (1%)	84	93
51	BN	95/95 (100%)	94 (99%)	1 (1%)	73	89
52	BO	186/186 (100%)	185 (100%)	1 (0%)	88	94
53	BP	104/104 (100%)	103 (99%)	1 (1%)	76	90
57	A	182/182 (100%)	181 (100%)	1 (0%)	88	94
58	B	172/173 (99%)	172 (100%)	0	100	100
59	C	88/89 (99%)	88 (100%)	0	100	100
60	D	89/98 (91%)	88 (99%)	1 (1%)	73	89
61	E	100/103 (97%)	100 (100%)	0	100	100
62	F	115/117 (98%)	114 (99%)	1 (1%)	78	91
63	G	113/113 (100%)	112 (99%)	1 (1%)	78	91
64	H	124/124 (100%)	124 (100%)	0	100	100
65	J	100/100 (100%)	99 (99%)	1 (1%)	76	90
66	K	61/61 (100%)	60 (98%)	1 (2%)	62	84
67	L	56/56 (100%)	56 (100%)	0	100	100
68	M	47/47 (100%)	47 (100%)	0	100	100
69	N	43/43 (100%)	43 (100%)	0	100	100
70	O	259/261 (99%)	259 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
71	P	177/184 (96%)	176 (99%)	1 (1%)	86 94
72	Q	191/191 (100%)	191 (100%)	0	100 100
73	R	180/180 (100%)	180 (100%)	0	100 100
74	S	219/221 (99%)	215 (98%)	4 (2%)	59 82
75	T	188/193 (97%)	187 (100%)	1 (0%)	88 94
76	U	160/165 (97%)	159 (99%)	1 (1%)	86 94
77	V	150/160 (94%)	149 (99%)	1 (1%)	84 93
78	W	152/152 (100%)	151 (99%)	1 (1%)	84 93
79	X	129/136 (95%)	128 (99%)	1 (1%)	81 92
80	Y	127/127 (100%)	126 (99%)	1 (1%)	81 92
81	Z	81/96 (84%)	81 (100%)	0	100 100
82	I	112/115 (97%)	112 (100%)	0	100 100
All	All	10005/10178 (98%)	9951 (100%)	54 (0%)	89 94

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AA	190	VAL
4	AC	68	ARG
11	AJ	104	ARG
12	AK	74	TYR
15	AN	121	ARG
18	AQ	23	GLN
19	AR	60	TYR
21	AT	17	ARG
24	AW	147	ARG
28	c	109	ARG
30	e	62	TYR
33	z	101	ARG
33	z	114	LYS
33	z	153	ASP
33	z	283	LEU
33	z	405	LYS
33	z	427	LYS
33	z	456	LYS
33	z	484	LYS
33	z	504	TYR
33	z	531	ARG

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Mol	Chain	Res	Type
33	z	601	LYS
33	z	652	LEU
33	z	746	PHE
33	z	790	LEU
33	z	824	LYS
33	z	886	LYS
33	z	897	LEU
38	BA	104	THR
38	BA	116	ARG
38	BA	332	ARG
46	BI	218	ARG
47	BJ	139	ARG
50	BM	46	ARG
51	BN	8	ARG
52	BO	93	ASN
53	BP	81	ARG
57	A	76	ARG
60	D	139	HIS
62	F	31	VAL
63	G	63	LYS
65	J	101	LYS
66	K	94	LYS
71	P	109	ASN
74	S	10	LYS
74	S	11	ARG
74	S	21	ASP
74	S	26	CYS
75	T	167	LYS
76	U	22	GLN
77	V	194	ARG
78	W	149	ARG
79	X	67	ARG
80	Y	138	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	AA	138	HIS
2	AA	252	ASN
5	AD	163	GLN
7	AF	30	GLN
8	AG	39	GLN

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Mol	Chain	Res	Type
10	AI	67	GLN
14	AM	126	GLN
17	AP	99	GLN
23	AV	12	GLN
24	AW	211	HIS
24	AW	215	ASN
27	b	15	ASN
33	z	37	ASN
33	z	73	GLN
33	z	96	GLN
33	z	200	HIS
33	z	349	ASN
33	z	602	ASN
38	BA	293	ASN
41	BD	207	ASN
42	BE	160	GLN
42	BE	291	ASN
44	BG	104	ASN
45	BH	65	ASN
46	BI	40	HIS
49	BL	9	GLN
50	BM	167	ASN
57	A	67	ASN
59	C	9	ASN
65	J	48	HIS
70	O	182	ASN
70	O	185	GLN
70	O	268	GLN
72	Q	74	GLN
75	T	201	GLN
76	U	110	GLN
77	V	35	ASN
77	V	87	ASN
80	Y	5	HIS
80	Y	105	ASN
82	I	23	GLN
82	I	101	ASN

5.3.3 RNA (i)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1763/1797 (98%)	508 (28%)	66 (3%)
34	l	16/17 (94%)	8 (50%)	0
35	n	75/76 (98%)	13 (17%)	0
36	m	74/75 (98%)	21 (28%)	0
54	BQ	3158/3396 (92%)	644 (20%)	92 (2%)
55	BR	120/121 (99%)	22 (18%)	3 (2%)
56	BS	157/158 (99%)	37 (23%)	4 (2%)
All	All	5363/5640 (95%)	1253 (23%)	165 (3%)

All (1253) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	34	G
1	2	39	A
1	2	41	A
1	2	42	G
1	2	47	A
1	2	49	C
1	2	50	C
1	2	51	A
1	2	52	U
1	2	53	G
1	2	55	A
1	2	56	U
1	2	57	G
1	2	60	U
1	2	62	A
1	2	63	G
1	2	66	U
1	2	68	A
1	2	69	G
1	2	71	A
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U

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Mol	Chain	Res	Type
1	2	76	A
1	2	78	A
1	2	79	C
1	2	81	G
1	2	93	A
1	2	99	C
1	2	104	A
1	2	105	A
1	2	106	U
1	2	114	C
1	2	121	U
1	2	126	A
1	2	129	U
1	2	130	C
1	2	131	C
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	138	A
1	2	140	A
1	2	141	U
1	2	142	G
1	2	153	G
1	2	155	U
1	2	159	U
1	2	161	U
1	2	168	A
1	2	171	A
1	2	174	U
1	2	175	G
1	2	176	C
1	2	178	U
1	2	180	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	189	C
1	2	191	C
1	2	193	U
1	2	195	G

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Mol	Chain	Res	Type
1	2	199	G
1	2	218	A
1	2	221	A
1	2	225	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	230	C
1	2	231	U
1	2	232	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	240	U
1	2	241	U
1	2	250	C
1	2	257	A
1	2	260	U
1	2	262	U
1	2	265	A
1	2	270	C
1	2	272	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	283	U
1	2	287	G
1	2	299	A
1	2	311	U
1	2	313	U
1	2	314	C
1	2	316	A
1	2	320	U
1	2	321	C
1	2	322	G
1	2	323	A
1	2	337	G
1	2	338	C
1	2	340	U
1	2	352	A
1	2	353	A
1	2	359	A

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Mol	Chain	Res	Type
1	2	361	C
1	2	370	A
1	2	373	G
1	2	379	U
1	2	380	U
1	2	381	C
1	2	383	G
1	2	384	G
1	2	385	A
1	2	388	G
1	2	390	G
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	405	C
1	2	415	C
1	2	417	A
1	2	419	G
1	2	423	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	429	G
1	2	430	G
1	2	434	G
1	2	436	A
1	2	439	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	453	U
1	2	454	U
1	2	455	C
1	2	460	A
1	2	468	A
1	2	471	A
1	2	477	A
1	2	486	G
1	2	489	C
1	2	492	A
1	2	493	U

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Mol	Chain	Res	Type
1	2	494	U
1	2	496	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	510	G
1	2	527	A
1	2	532	U
1	2	534	A
1	2	538	A
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	548	G
1	2	549	G
1	2	555	A
1	2	556	A
1	2	557	G
1	2	559	C
1	2	565	C
1	2	578	U
1	2	579	A
1	2	580	A
1	2	582	U
1	2	594	A
1	2	595	G
1	2	597	G
1	2	606	A
1	2	610	G
1	2	611	U
1	2	619	A
1	2	620	A
1	2	623	A
1	2	624	G
1	2	634	G
1	2	638	U

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Mol	Chain	Res	Type
1	2	639	U
1	2	640	U
1	2	643	G
1	2	644	C
1	2	650	U
1	2	651	G
1	2	652	G
1	2	653	C
1	2	655	G
1	2	657	U
1	2	658	C
1	2	678	A
1	2	679	U
1	2	680	U
1	2	681	U
1	2	682	C
1	2	683	C
1	2	684	A
1	2	694	U
1	2	696	C
1	2	698	U
1	2	699	U
1	2	700	C
1	2	704	C
1	2	705	U
1	2	706	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	711	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	715	U
1	2	716	C
1	2	717	C
1	2	718	U
1	2	719	U
1	2	721	U
1	2	723	G
1	2	725	U
1	2	726	C

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Mol	Chain	Res	Type
1	2	727	U
1	2	729	G
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	738	G
1	2	739	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	744	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	767	U
1	2	768	C
1	2	774	A
1	2	775	G
1	2	776	G
1	2	778	G
1	2	780	A
1	2	782	U
1	2	783	G
1	2	789	A
1	2	811	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	816	G
1	2	817	A
1	2	818	C
1	2	820	U
1	2	821	U
1	2	823	G
1	2	833	U
1	2	834	G

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Mol	Chain	Res	Type
1	2	838	G
1	2	840	U
1	2	846	G
1	2	856	A
1	2	857	U
1	2	863	A
1	2	864	U
1	2	876	G
1	2	886	U
1	2	898	A
1	2	899	G
1	2	913	G
1	2	914	G
1	2	928	U
1	2	929	A
1	2	933	A
1	2	934	C
1	2	935	U
1	2	942	G
1	2	944	A
1	2	960	U
1	2	964	U
1	2	966	A
1	2	970	A
1	2	984	G
1	2	988	A
1	2	992	A
1	2	993	A
1	2	1024	U
1	2	1026	A
1	2	1028	C
1	2	1030	A
1	2	1031	U
1	2	1032	G
1	2	1039	A
1	2	1053	G
1	2	1057	U
1	2	1058	U
1	2	1061	A
1	2	1076	A
1	2	1082	C
1	2	1086	A

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Mol	Chain	Res	Type
1	2	1092	A
1	2	1096	C
1	2	1098	U
1	2	1099	U
1	2	1100	G
1	2	1113	A
1	2	1114	G
1	2	1115	U
1	2	1138	A
1	2	1150	G
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1170	G
1	2	1172	G
1	2	1174	C
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1199	G
1	2	1200	G
1	2	1208	A
1	2	1217	A
1	2	1218	G
1	2	1227	A
1	2	1229	G
1	2	1241	G
1	2	1242	A
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1247	U
1	2	1251	U
1	2	1252	C
1	2	1256	A
1	2	1257	U
1	2	1258	U
1	2	1273	G
1	2	1274	C

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Mol	Chain	Res	Type
1	2	1275	A
1	2	1285	U
1	2	1294	G
1	2	1301	U
1	2	1307	U
1	2	1314	U
1	2	1315	U
1	2	1318	G
1	2	1321	A
1	2	1322	A
1	2	1337	A
1	2	1338	C
1	2	1339	C
1	2	1340	U
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1347	U
1	2	1348	A
1	2	1349	G
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1367	G
1	2	1370	U
1	2	1371	A
1	2	1373	C
1	2	1378	U
1	2	1381	U
1	2	1382	A
1	2	1383	G
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1402	G
1	2	1410	A
1	2	1412	G
1	2	1414	U
1	2	1415	U
1	2	1425	A
1	2	1427	A

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Mol	Chain	Res	Type
1	2	1431	C
1	2	1432	U
1	2	1437	U
1	2	1444	A
1	2	1445	G
1	2	1446	A
1	2	1447	C
1	2	1448	G
1	2	1458	G
1	2	1459	C
1	2	1465	C
1	2	1466	G
1	2	1468	U
1	2	1469	A
1	2	1470	C
1	2	1471	A
1	2	1472	C
1	2	1473	U
1	2	1476	C
1	2	1477	G
1	2	1478	G
1	2	1480	G
1	2	1481	C
1	2	1482	C
1	2	1483	A
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1496	U
1	2	1506	G
1	2	1516	A
1	2	1518	C
1	2	1521	G
1	2	1522	U
1	2	1524	A
1	2	1527	C
1	2	1528	U
1	2	1529	C
1	2	1531	G
1	2	1535	U
1	2	1536	G
1	2	1537	C

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Mol	Chain	Res	Type
1	2	1538	U
1	2	1540	G
1	2	1541	G
1	2	1543	A
1	2	1544	U
1	2	1554	U
1	2	1557	U
1	2	1558	U
1	2	1559	A
1	2	1571	C
1	2	1572	G
1	2	1574	G
1	2	1575	G
1	2	1576	A
1	2	1577	A
1	2	1584	G
1	2	1585	U
1	2	1590	G
1	2	1601	G
1	2	1602	C
1	2	1605	G
1	2	1607	G
1	2	1611	A
1	2	1616	G
1	2	1622	G
1	2	1631	A
1	2	1634	C
1	2	1635	A
1	2	1637	C
1	2	1639	C
1	2	1657	U
1	2	1658	G
1	2	1682	U
1	2	1688	U
1	2	1689	A
1	2	1693	A
1	2	1709	C
1	2	1711	C
1	2	1712	A
1	2	1715	G
1	2	1736	G
1	2	1757	G

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Mol	Chain	Res	Type
1	2	1760	G
1	2	1762	A
1	2	1765	A
1	2	1766	A
1	2	1767	G
1	2	1768	G
1	2	1769	U
1	2	1770	U
1	2	1771	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
34	l	33	A
34	l	35	C
34	l	36	C
34	l	37	U
34	l	38	G
34	l	40	A
34	l	42	G
34	l	46	C
35	n	16	U
35	n	17	G
35	n	19	U
35	n	24	G
35	n	32	C
35	n	41	A
35	n	42	G
35	n	47	U
35	n	48	U
35	n	58	A
35	n	59	G
35	n	73	G
35	n	76	A
36	m	16	C
36	m	17	G
36	m	18	G
36	m	19	C

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Mol	Chain	Res	Type
36	m	21	A
36	m	28	C
36	m	29	A
36	m	33	U
36	m	34	U
36	m	36	C
36	m	37	A
36	m	38	C
36	m	39	C
36	m	42	G
36	m	43	G
36	m	45	G
36	m	46	A
36	m	55	C
36	m	59	U
36	m	72	G
36	m	75	A
54	BQ	13	A
54	BQ	14	U
54	BQ	26	A
54	BQ	30	G
54	BQ	40	A
54	BQ	43	A
54	BQ	45	A
54	BQ	49	A
54	BQ	59	G
54	BQ	60	A
54	BQ	65	A
54	BQ	66	A
54	BQ	73	C
54	BQ	77	A
54	BQ	83	U
54	BQ	85	A
54	BQ	86	G
54	BQ	87	U
54	BQ	92	G
54	BQ	111	C
54	BQ	119	U
54	BQ	120	G
54	BQ	122	A
54	BQ	134	U
54	BQ	135	C

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Mol	Chain	Res	Type
54	BQ	136	G
54	BQ	146	U
54	BQ	147	U
54	BQ	148	G
54	BQ	155	G
54	BQ	156	G
54	BQ	157	A
54	BQ	161	G
54	BQ	165	A
54	BQ	166	C
54	BQ	168	U
54	BQ	187	A
54	BQ	188	U
54	BQ	189	G
54	BQ	190	U
54	BQ	191	U
54	BQ	200	C
54	BQ	206	G
54	BQ	210	U
54	BQ	211	A
54	BQ	212	G
54	BQ	213	A
54	BQ	218	G
54	BQ	219	A
54	BQ	221	A
54	BQ	222	A
54	BQ	234	G
54	BQ	240	U
54	BQ	241	G
54	BQ	244	G
54	BQ	249	U
54	BQ	251	G
54	BQ	252	U
54	BQ	253	A
54	BQ	269	G
54	BQ	270	U
54	BQ	283	G
54	BQ	286	U
54	BQ	295	A
54	BQ	298	U
54	BQ	311	C
54	BQ	323	A

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Mol	Chain	Res	Type
54	BQ	329	U
54	BQ	330	G
54	BQ	334	A
54	BQ	346	C
54	BQ	352	A
54	BQ	375	A
54	BQ	376	G
54	BQ	395	A
54	BQ	398	A
54	BQ	399	A
54	BQ	401	U
54	BQ	402	A
54	BQ	403	C
54	BQ	421	G
54	BQ	422	A
54	BQ	429	U
54	BQ	440	A
54	BQ	495	G
54	BQ	507	U
54	BQ	510	G
54	BQ	521	A
54	BQ	523	A
54	BQ	525	C
54	BQ	533	A
54	BQ	535	G
54	BQ	544	C
54	BQ	546	C
54	BQ	547	G
54	BQ	548	G
54	BQ	549	U
54	BQ	550	A
54	BQ	551	A
54	BQ	556	U
54	BQ	557	A
54	BQ	559	A
54	BQ	578	A
54	BQ	579	G
54	BQ	592	A
54	BQ	600	G
54	BQ	604	G
54	BQ	609	G
54	BQ	612	U

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Mol	Chain	Res	Type
54	BQ	620	U
54	BQ	621	A
54	BQ	622	A
54	BQ	636	C
54	BQ	637	C
54	BQ	649	A
54	BQ	660	A
54	BQ	667	C
54	BQ	671	U
54	BQ	675	C
54	BQ	677	A
54	BQ	678	G
54	BQ	681	U
54	BQ	684	G
54	BQ	690	A
54	BQ	691	A
54	BQ	692	A
54	BQ	705	A
54	BQ	712	G
54	BQ	715	A
54	BQ	716	A
54	BQ	719	U
54	BQ	720	A
54	BQ	735	A
54	BQ	758	C
54	BQ	764	U
54	BQ	765	C
54	BQ	766	U
54	BQ	767	U
54	BQ	768	C
54	BQ	777	U
54	BQ	780	A
54	BQ	781	G
54	BQ	784	A
54	BQ	785	G
54	BQ	786	A
54	BQ	800	G
54	BQ	801	A
54	BQ	806	A
54	BQ	816	A
54	BQ	817	A
54	BQ	830	A

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Mol	Chain	Res	Type
54	BQ	849	C
54	BQ	861	C
54	BQ	867	G
54	BQ	874	U
54	BQ	879	U
54	BQ	885	U
54	BQ	895	A
54	BQ	896	A
54	BQ	907	G
54	BQ	908	G
54	BQ	914	A
54	BQ	916	G
54	BQ	917	A
54	BQ	923	C
54	BQ	926	A
54	BQ	934	G
54	BQ	937	G
54	BQ	944	C
54	BQ	953	G
54	BQ	959	C
54	BQ	960	U
54	BQ	974	G
54	BQ	980	A
54	BQ	981	U
54	BQ	994	G
54	BQ	995	U
54	BQ	1001	G
54	BQ	1005	G
54	BQ	1010	G
54	BQ	1015	U
54	BQ	1016	C
54	BQ	1017	C
54	BQ	1018	G
54	BQ	1028	U
54	BQ	1029	G
54	BQ	1030	A
54	BQ	1032	C
54	BQ	1036	A
54	BQ	1041	U
54	BQ	1047	A
54	BQ	1049	C
54	BQ	1065	A

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Mol	Chain	Res	Type
54	BQ	1072	G
54	BQ	1076	C
54	BQ	1081	U
54	BQ	1082	U
54	BQ	1083	G
54	BQ	1093	A
54	BQ	1095	U
54	BQ	1096	U
54	BQ	1097	G
54	BQ	1098	A
54	BQ	1103	A
54	BQ	1104	G
54	BQ	1117	G
54	BQ	1131	G
54	BQ	1135	A
54	BQ	1144	U
54	BQ	1145	G
54	BQ	1153	A
54	BQ	1155	C
54	BQ	1159	A
54	BQ	1180	A
54	BQ	1181	U
54	BQ	1191	U
54	BQ	1192	C
54	BQ	1197	A
54	BQ	1200	A
54	BQ	1201	C
54	BQ	1202	A
54	BQ	1206	G
54	BQ	1217	A
54	BQ	1219	C
54	BQ	1221	A
54	BQ	1222	G
54	BQ	1225	A
54	BQ	1230	G
54	BQ	1233	G
54	BQ	1235	U
54	BQ	1236	G
54	BQ	1237	G
54	BQ	1238	C
54	BQ	1239	C
54	BQ	1241	U

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Mol	Chain	Res	Type
54	BQ	1245	A
54	BQ	1246	G
54	BQ	1248	C
54	BQ	1250	G
54	BQ	1252	A
54	BQ	1253	U
54	BQ	1254	C
54	BQ	1257	C
54	BQ	1260	A
54	BQ	1262	G
54	BQ	1263	A
54	BQ	1264	G
54	BQ	1265	U
54	BQ	1266	G
54	BQ	1268	G
54	BQ	1270	A
54	BQ	1271	A
54	BQ	1272	C
54	BQ	1274	A
54	BQ	1276	U
54	BQ	1281	G
54	BQ	1282	G
54	BQ	1286	A
54	BQ	1287	A
54	BQ	1294	A
54	BQ	1301	A
54	BQ	1303	A
54	BQ	1307	G
54	BQ	1308	A
54	BQ	1309	U
54	BQ	1313	G
54	BQ	1315	U
54	BQ	1316	C
54	BQ	1325	U
54	BQ	1330	A
54	BQ	1331	U
54	BQ	1345	G
54	BQ	1348	U
54	BQ	1350	A
54	BQ	1351	U
54	BQ	1352	A
54	BQ	1355	A

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Mol	Chain	Res	Type
54	BQ	1356	U
54	BQ	1357	G
54	BQ	1380	G
54	BQ	1386	A
54	BQ	1392	G
54	BQ	1399	A
54	BQ	1400	G
54	BQ	1408	G
54	BQ	1418	A
54	BQ	1419	A
54	BQ	1421	G
54	BQ	1434	G
54	BQ	1437	C
54	BQ	1443	G
54	BQ	1446	A
54	BQ	1447	G
54	BQ	1448	U
54	BQ	1450	G
54	BQ	1456	A
54	BQ	1475	A
54	BQ	1481	A
54	BQ	1482	A
54	BQ	1483	G
54	BQ	1484	U
54	BQ	1485	G
54	BQ	1487	G
54	BQ	1503	A
54	BQ	1508	C
54	BQ	1523	U
54	BQ	1528	G
54	BQ	1533	U
54	BQ	1536	G
54	BQ	1542	G
54	BQ	1554	U
54	BQ	1555	U
54	BQ	1556	C
54	BQ	1557	A
54	BQ	1559	A
54	BQ	1560	G
54	BQ	1561	G
54	BQ	1563	C
54	BQ	1565	G

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Mol	Chain	Res	Type
54	BQ	1566	A
54	BQ	1567	U
54	BQ	1568	U
54	BQ	1569	U
54	BQ	1570	U
54	BQ	1571	A
54	BQ	1572	U
54	BQ	1573	G
54	BQ	1576	G
54	BQ	1579	C
54	BQ	1580	A
54	BQ	1581	C
54	BQ	1582	C
54	BQ	1583	A
54	BQ	1588	A
54	BQ	1589	A
54	BQ	1593	A
54	BQ	1605	A
54	BQ	1620	U
54	BQ	1629	U
54	BQ	1630	U
54	BQ	1631	C
54	BQ	1642	A
54	BQ	1643	A
54	BQ	1645	U
54	BQ	1646	G
54	BQ	1657	C
54	BQ	1683	A
54	BQ	1714	A
54	BQ	1724	U
54	BQ	1729	A
54	BQ	1730	G
54	BQ	1741	A
54	BQ	1750	A
54	BQ	1751	G
54	BQ	1752	A
54	BQ	1760	A
54	BQ	1762	C
54	BQ	1763	U
54	BQ	1765	U
54	BQ	1766	G
54	BQ	1770	G

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Mol	Chain	Res	Type
54	BQ	1780	G
54	BQ	1797	A
54	BQ	1809	A
54	BQ	1813	A
54	BQ	1814	A
54	BQ	1815	U
54	BQ	1816	A
54	BQ	1817	G
54	BQ	1818	U
54	BQ	1819	U
54	BQ	1820	U
54	BQ	1821	U
54	BQ	1835	A
54	BQ	1839	A
54	BQ	1840	U
54	BQ	1841	A
54	BQ	1845	G
54	BQ	1846	C
54	BQ	1849	C
54	BQ	1850	A
54	BQ	1866	C
54	BQ	1868	G
54	BQ	1879	A
54	BQ	1880	U
54	BQ	1885	U
54	BQ	1886	A
54	BQ	1893	A
54	BQ	1900	A
54	BQ	1901	A
54	BQ	1906	G
54	BQ	1914	G
54	BQ	1920	U
54	BQ	1930	A
54	BQ	1932	A
54	BQ	1952	G
54	BQ	1953	G
54	BQ	1954	G
54	BQ	2094	C
54	BQ	2101	C
54	BQ	2102	U
54	BQ	2107	A
54	BQ	2111	G

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Mol	Chain	Res	Type
54	BQ	2112	U
54	BQ	2113	A
54	BQ	2114	C
54	BQ	2121	G
54	BQ	2122	G
54	BQ	2131	A
54	BQ	2139	A
54	BQ	2158	A
54	BQ	2159	U
54	BQ	2169	G
54	BQ	2170	U
54	BQ	2179	C
54	BQ	2188	A
54	BQ	2197	C
54	BQ	2201	G
54	BQ	2205	U
54	BQ	2206	G
54	BQ	2209	U
54	BQ	2210	G
54	BQ	2243	A
54	BQ	2244	A
54	BQ	2249	G
54	BQ	2256	A
54	BQ	2257	C
54	BQ	2272	G
54	BQ	2273	G
54	BQ	2274	U
54	BQ	2281	A
54	BQ	2282	U
54	BQ	2284	C
54	BQ	2307	G
54	BQ	2310	U
54	BQ	2313	A
54	BQ	2314	U
54	BQ	2315	G
54	BQ	2334	U
54	BQ	2336	U
54	BQ	2340	U
54	BQ	2373	A
54	BQ	2374	C
54	BQ	2375	G
54	BQ	2376	G

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Mol	Chain	Res	Type
54	BQ	2388	U
54	BQ	2393	G
54	BQ	2397	A
54	BQ	2398	A
54	BQ	2402	A
54	BQ	2403	G
54	BQ	2404	A
54	BQ	2411	U
54	BQ	2419	A
54	BQ	2434	U
54	BQ	2435	G
54	BQ	2437	G
54	BQ	2439	A
54	BQ	2444	C
54	BQ	2446	U
54	BQ	2451	G
54	BQ	2496	C
54	BQ	2498	U
54	BQ	2501	U
54	BQ	2502	A
54	BQ	2514	U
54	BQ	2515	A
54	BQ	2522	G
54	BQ	2523	A
54	BQ	2524	A
54	BQ	2530	G
54	BQ	2531	C
54	BQ	2538	U
54	BQ	2540	A
54	BQ	2541	U
54	BQ	2542	U
54	BQ	2549	G
54	BQ	2552	C
54	BQ	2553	U
54	BQ	2554	A
54	BQ	2560	C
54	BQ	2562	A
54	BQ	2570	U
54	BQ	2571	U
54	BQ	2572	C
54	BQ	2585	G
54	BQ	2586	G

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Mol	Chain	Res	Type
54	BQ	2593	A
54	BQ	2594	C
54	BQ	2606	G
54	BQ	2607	G
54	BQ	2619	G
54	BQ	2627	C
54	BQ	2635	A
54	BQ	2652	U
54	BQ	2656	A
54	BQ	2666	C
54	BQ	2674	A
54	BQ	2677	G
54	BQ	2679	A
54	BQ	2681	U
54	BQ	2689	A
54	BQ	2691	A
54	BQ	2694	A
54	BQ	2703	A
54	BQ	2704	A
54	BQ	2714	G
54	BQ	2716	U
54	BQ	2727	A
54	BQ	2728	G
54	BQ	2729	U
54	BQ	2737	C
54	BQ	2740	A
54	BQ	2742	C
54	BQ	2753	G
54	BQ	2762	A
54	BQ	2772	C
54	BQ	2777	G
54	BQ	2778	G
54	BQ	2800	G
54	BQ	2801	A
54	BQ	2802	A
54	BQ	2804	A
54	BQ	2810	C
54	BQ	2816	G
54	BQ	2817	A
54	BQ	2842	U
54	BQ	2845	A
54	BQ	2847	A

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Mol	Chain	Res	Type
54	BQ	2860	U
54	BQ	2867	C
54	BQ	2871	G
54	BQ	2872	A
54	BQ	2887	A
54	BQ	2888	U
54	BQ	2889	C
54	BQ	2894	C
54	BQ	2898	G
54	BQ	2911	A
54	BQ	2912	G
54	BQ	2914	G
54	BQ	2915	U
54	BQ	2923	U
54	BQ	2928	C
54	BQ	2935	U
54	BQ	2936	A
54	BQ	2938	G
54	BQ	2941	A
54	BQ	2942	C
54	BQ	2945	G
54	BQ	2947	G
54	BQ	2971	A
54	BQ	2972	G
54	BQ	2977	G
54	BQ	2978	U
54	BQ	2979	U
54	BQ	2983	C
54	BQ	2990	G
54	BQ	2996	U
54	BQ	2997	G
54	BQ	3012	A
54	BQ	3022	G
54	BQ	3023	U
54	BQ	3049	A
54	BQ	3055	U
54	BQ	3056	U
54	BQ	3058	U
54	BQ	3078	U
54	BQ	3080	G
54	BQ	3086	A
54	BQ	3092	C

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Mol	Chain	Res	Type
54	BQ	3117	C
54	BQ	3128	G
54	BQ	3130	A
54	BQ	3131	U
54	BQ	3141	A
54	BQ	3142	A
54	BQ	3143	C
54	BQ	3151	U
54	BQ	3152	U
54	BQ	3153	U
54	BQ	3154	C
54	BQ	3156	U
54	BQ	3157	U
54	BQ	3158	G
54	BQ	3170	A
54	BQ	3172	A
54	BQ	3174	A
54	BQ	3176	G
54	BQ	3179	U
54	BQ	3180	A
54	BQ	3181	C
54	BQ	3186	A
54	BQ	3187	A
54	BQ	3206	C
54	BQ	3207	U
54	BQ	3208	G
54	BQ	3210	A
54	BQ	3217	C
54	BQ	3218	A
54	BQ	3220	G
54	BQ	3224	G
54	BQ	3241	G
54	BQ	3242	G
54	BQ	3243	A
54	BQ	3245	A
54	BQ	3247	G
54	BQ	3259	U
54	BQ	3260	G
54	BQ	3263	G
54	BQ	3268	A
54	BQ	3270	U
54	BQ	3271	G

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Mol	Chain	Res	Type
54	BQ	3272	C
54	BQ	3276	G
54	BQ	3277	U
54	BQ	3279	A
54	BQ	3287	U
54	BQ	3289	G
54	BQ	3294	A
54	BQ	3295	A
54	BQ	3304	U
54	BQ	3313	U
54	BQ	3316	A
54	BQ	3318	G
54	BQ	3319	U
54	BQ	3345	G
54	BQ	3346	U
54	BQ	3347	A
54	BQ	3348	G
54	BQ	3349	C
54	BQ	3351	U
54	BQ	3352	U
54	BQ	3353	G
54	BQ	3354	U
54	BQ	3355	U
54	BQ	3356	G
54	BQ	3369	G
54	BQ	3375	A
54	BQ	3378	C
54	BQ	3382	U
54	BQ	3383	G
54	BQ	3386	G
54	BQ	3390	G
55	BR	7	G
55	BR	11	A
55	BR	13	A
55	BR	22	A
55	BR	29	C
55	BR	33	U
55	BR	42	A
55	BR	49	G
55	BR	50	U
55	BR	55	A
55	BR	65	G

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Mol	Chain	Res	Type
55	BR	74	C
55	BR	76	A
55	BR	77	G
55	BR	78	U
55	BR	79	A
55	BR	87	G
55	BR	91	G
55	BR	102	A
55	BR	104	A
55	BR	112	G
55	BR	121	U
56	BS	17	A
56	BS	22	U
56	BS	23	U
56	BS	34	U
56	BS	35	C
56	BS	52	A
56	BS	53	A
56	BS	59	A
56	BS	60	U
56	BS	62	C
56	BS	63	G
56	BS	71	A
56	BS	80	A
56	BS	82	U
56	BS	83	C
56	BS	84	C
56	BS	85	G
56	BS	86	U
56	BS	90	U
56	BS	91	C
56	BS	95	G
56	BS	97	A
56	BS	102	U
56	BS	104	A
56	BS	105	A
56	BS	106	C
56	BS	112	U
56	BS	113	U
56	BS	116	G
56	BS	125	U
56	BS	126	A

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Mol	Chain	Res	Type
56	BS	129	C
56	BS	144	G
56	BS	148	G
56	BS	151	C
56	BS	152	G
56	BS	157	U

All (165) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	52	U
1	2	68	A
1	2	77	U
1	2	80	A
1	2	132	U
1	2	139	C
1	2	170	U
1	2	174	U
1	2	217	A
1	2	224	C
1	2	228	G
1	2	261	U
1	2	278	U
1	2	312	A
1	2	313	U
1	2	321	C
1	2	322	G
1	2	352	A
1	2	380	U
1	2	387	A
1	2	400	A
1	2	423	G
1	2	454	U
1	2	539	G
1	2	541	A
1	2	555	A
1	2	609	U
1	2	639	U
1	2	705	U
1	2	711	U
1	2	714	G
1	2	754	A

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Mol	Chain	Res	Type
1	2	755	A
1	2	765	G
1	2	766	U
1	2	819	G
1	2	863	A
1	2	928	U
1	2	1023	A
1	2	1108	G
1	2	1114	G
1	2	1216	C
1	2	1217	A
1	2	1226	A
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1251	U
1	2	1256	A
1	2	1273	G
1	2	1274	C
1	2	1344	A
1	2	1373	C
1	2	1382	A
1	2	1399	C
1	2	1413	U
1	2	1430	U
1	2	1465	C
1	2	1469	A
1	2	1535	U
1	2	1540	G
1	2	1556	A
1	2	1573	A
1	2	1584	G
1	2	1633	A
1	2	1636	C
54	BQ	13	A
54	BQ	40	A
54	BQ	86	G
54	BQ	154	U
54	BQ	155	G
54	BQ	211	A
54	BQ	221	A
54	BQ	269	G

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Mol	Chain	Res	Type
54	BQ	282	G
54	BQ	297	G
54	BQ	374	A
54	BQ	400	G
54	BQ	520	U
54	BQ	547	G
54	BQ	588	G
54	BQ	677	A
54	BQ	764	U
54	BQ	767	U
54	BQ	784	A
54	BQ	800	G
54	BQ	896	A
54	BQ	916	G
54	BQ	925	A
54	BQ	979	U
54	BQ	993	G
54	BQ	1064	A
54	BQ	1095	U
54	BQ	1103	A
54	BQ	1144	U
54	BQ	1307	G
54	BQ	1315	U
54	BQ	1355	A
54	BQ	1417	G
54	BQ	1447	G
54	BQ	1481	A
54	BQ	1483	G
54	BQ	1553	U
54	BQ	1554	U
54	BQ	1558	A
54	BQ	1572	U
54	BQ	1580	A
54	BQ	1642	A
54	BQ	1657	C
54	BQ	1713	G
54	BQ	1729	A
54	BQ	1751	G
54	BQ	1808	G
54	BQ	1815	U
54	BQ	1816	A
54	BQ	1820	U

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Mol	Chain	Res	Type
54	BQ	1839	A
54	BQ	1840	U
54	BQ	1900	A
54	BQ	1913	A
54	BQ	2101	C
54	BQ	2112	U
54	BQ	2138	A
54	BQ	2178	A
54	BQ	2208	A
54	BQ	2273	G
54	BQ	2281	A
54	BQ	2283	G
54	BQ	2434	U
54	BQ	2445	A
54	BQ	2495	C
54	BQ	2500	A
54	BQ	2501	U
54	BQ	2513	U
54	BQ	2514	U
54	BQ	2523	A
54	BQ	2541	U
54	BQ	2593	A
54	BQ	2665	U
54	BQ	2680	A
54	BQ	2727	A
54	BQ	2816	G
54	BQ	2941	A
54	BQ	2971	A
54	BQ	3022	G
54	BQ	3140	G
54	BQ	3156	U
54	BQ	3175	U
54	BQ	3219	G
54	BQ	3242	G
54	BQ	3243	A
54	BQ	3269	U
54	BQ	3293	U
54	BQ	3345	G
54	BQ	3350	C
54	BQ	3353	G
54	BQ	3355	U
54	BQ	3382	U

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Mol	Chain	Res	Type
55	BR	41	G
55	BR	77	G
55	BR	86	U
56	BS	16	G
56	BS	22	U
56	BS	85	G
56	BS	105	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

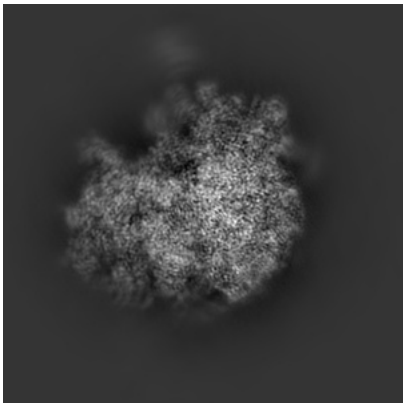
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4474. These allow visual inspection of the internal detail of the map and identification of artifacts.

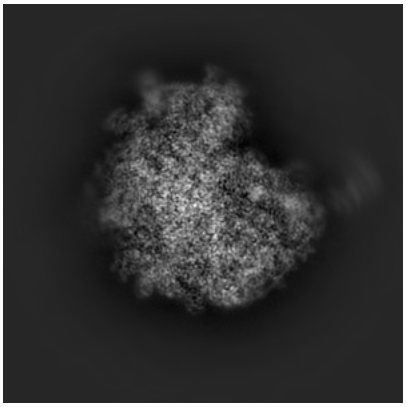
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

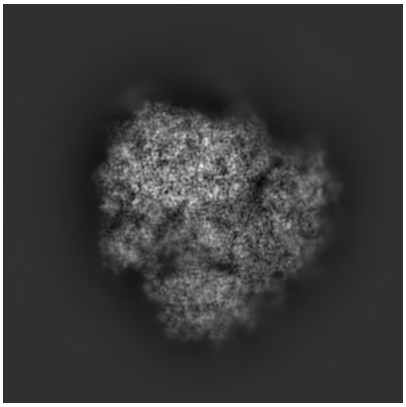
6.1.1 Primary map



X



Y

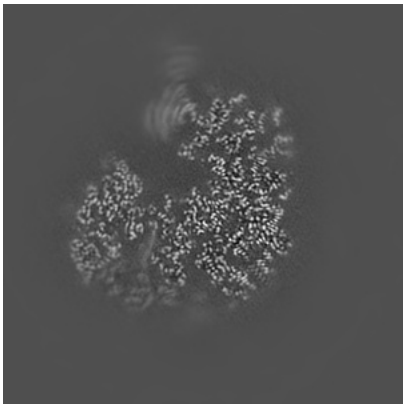


Z

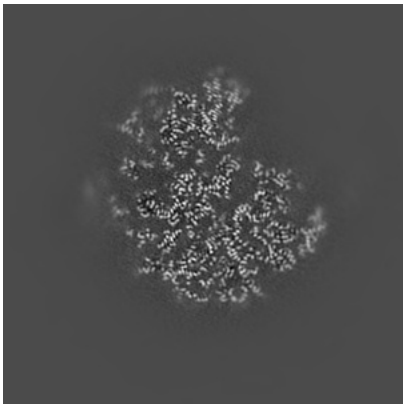
The images above show the map projected in three orthogonal directions.

6.2 Central slices

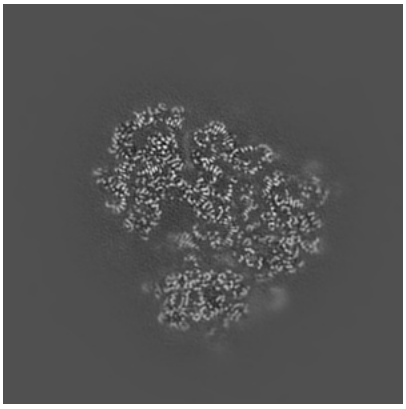
6.2.1 Primary map



X Index: 200



Y Index: 200

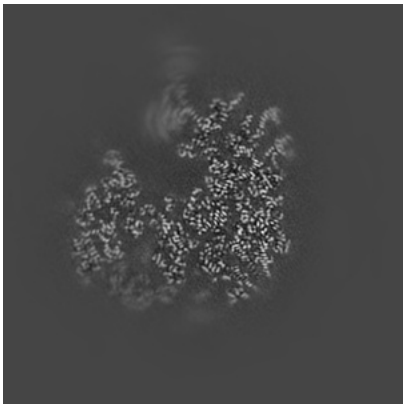


Z Index: 200

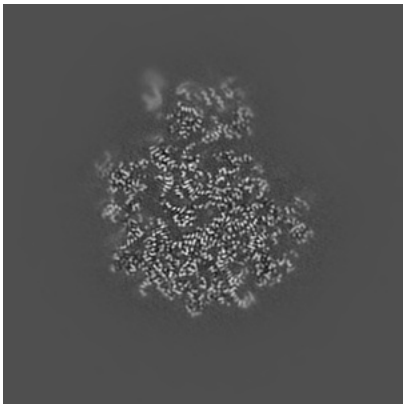
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

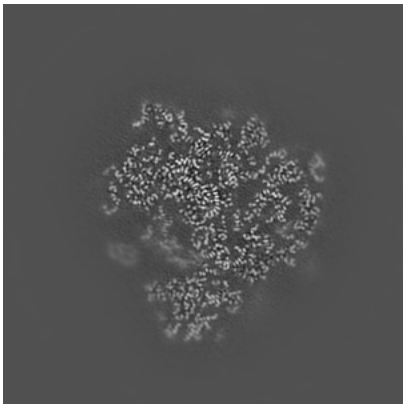
6.3.1 Primary map



X Index: 203



Y Index: 226



Z Index: 180

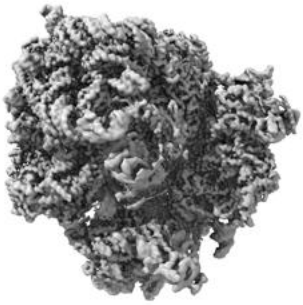
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

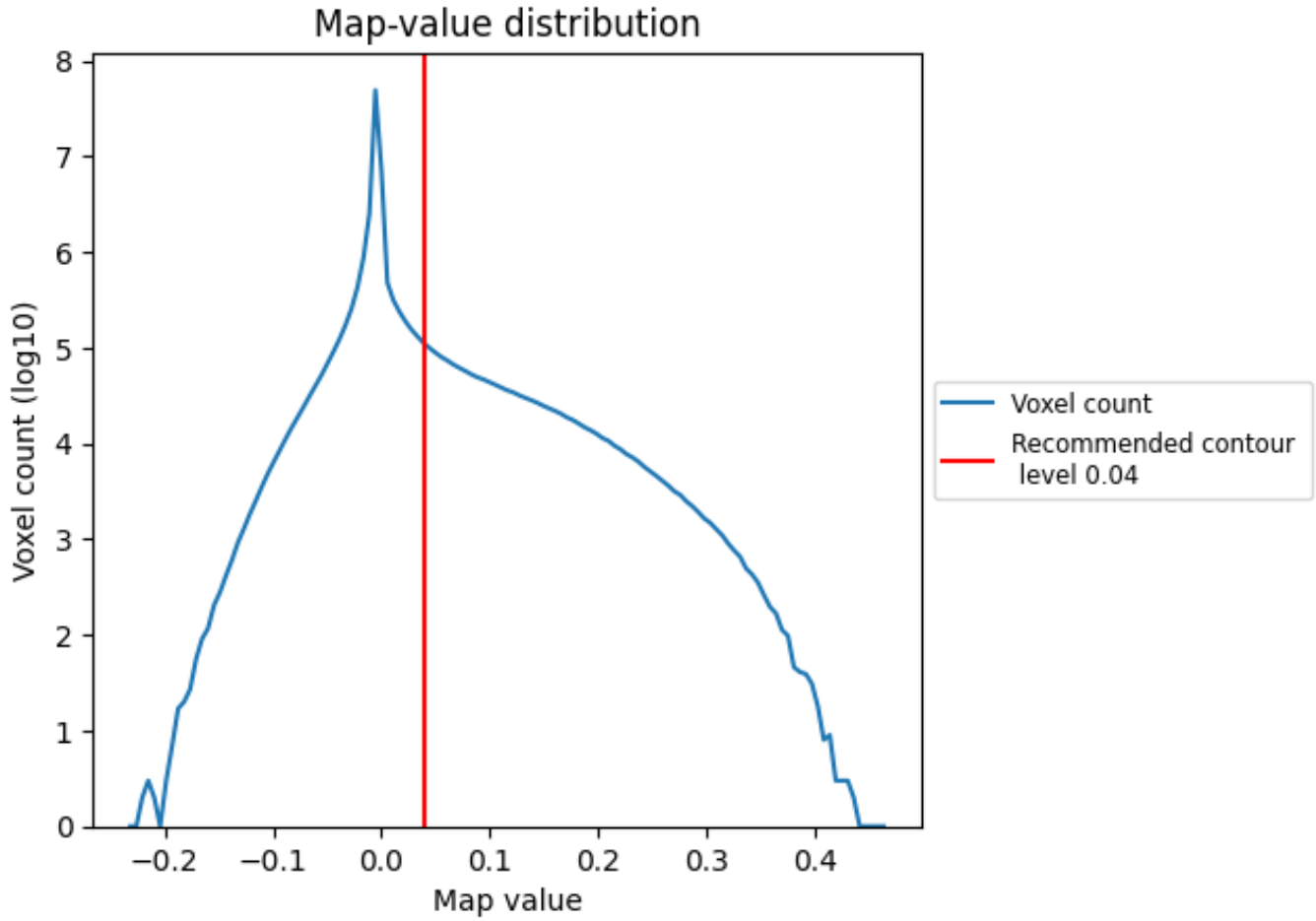
6.5 Mask visualisation (i)

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

7 Map analysis

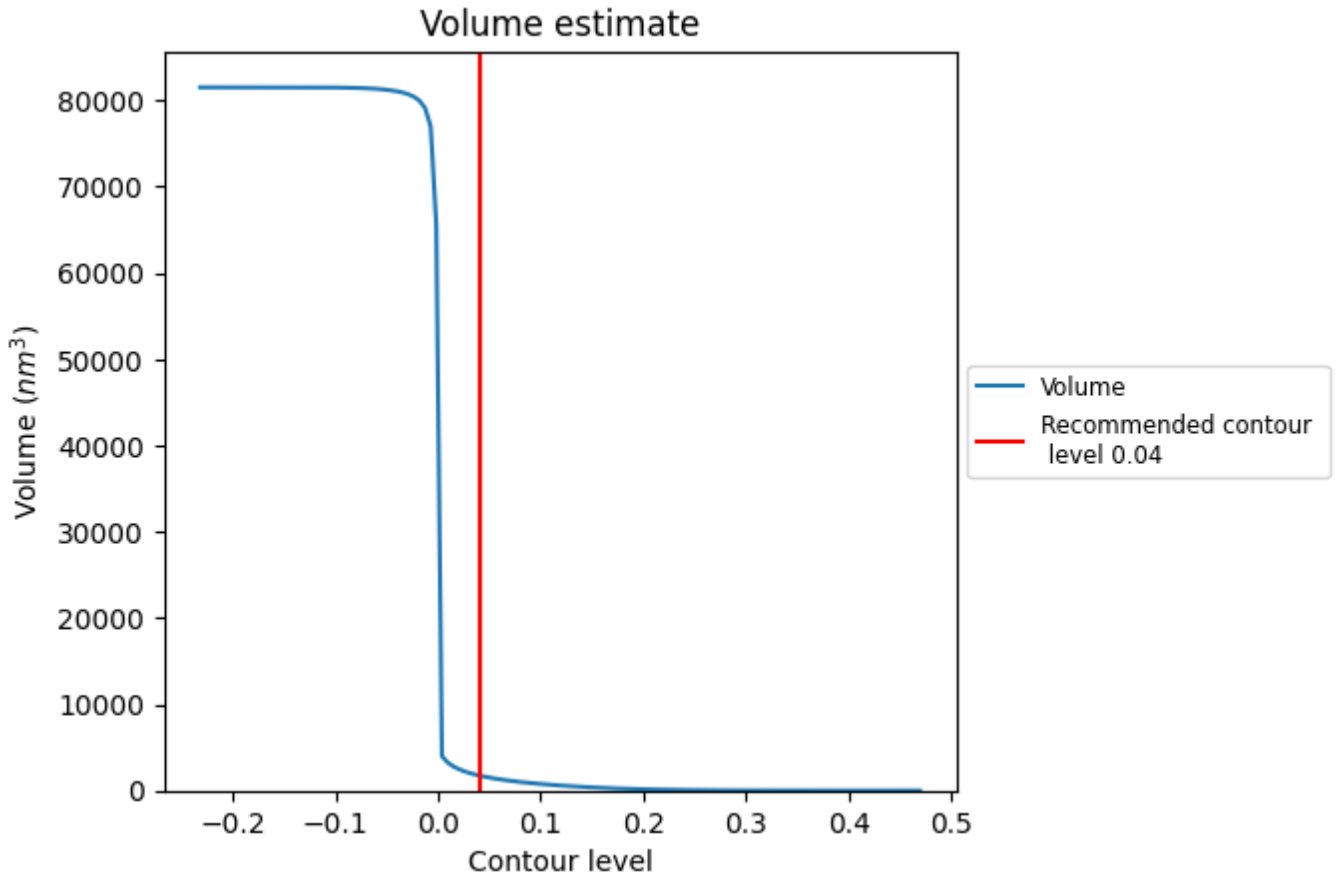
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

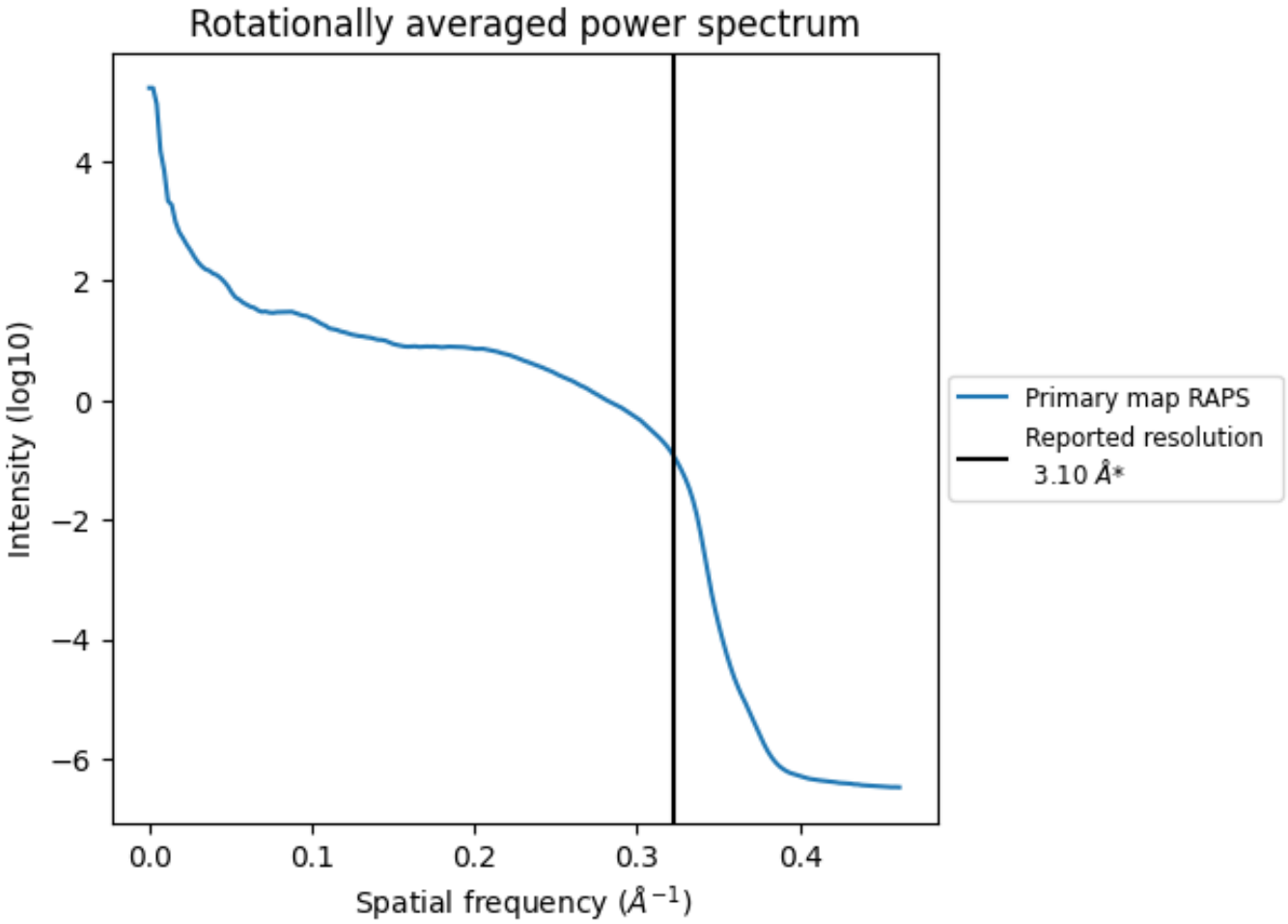
7.2 Volume estimate



The volume at the recommended contour level is 1744 nm^3; this corresponds to an approximate mass of 1575 kDa.

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

7.3 Rotationally averaged power spectrum (i)

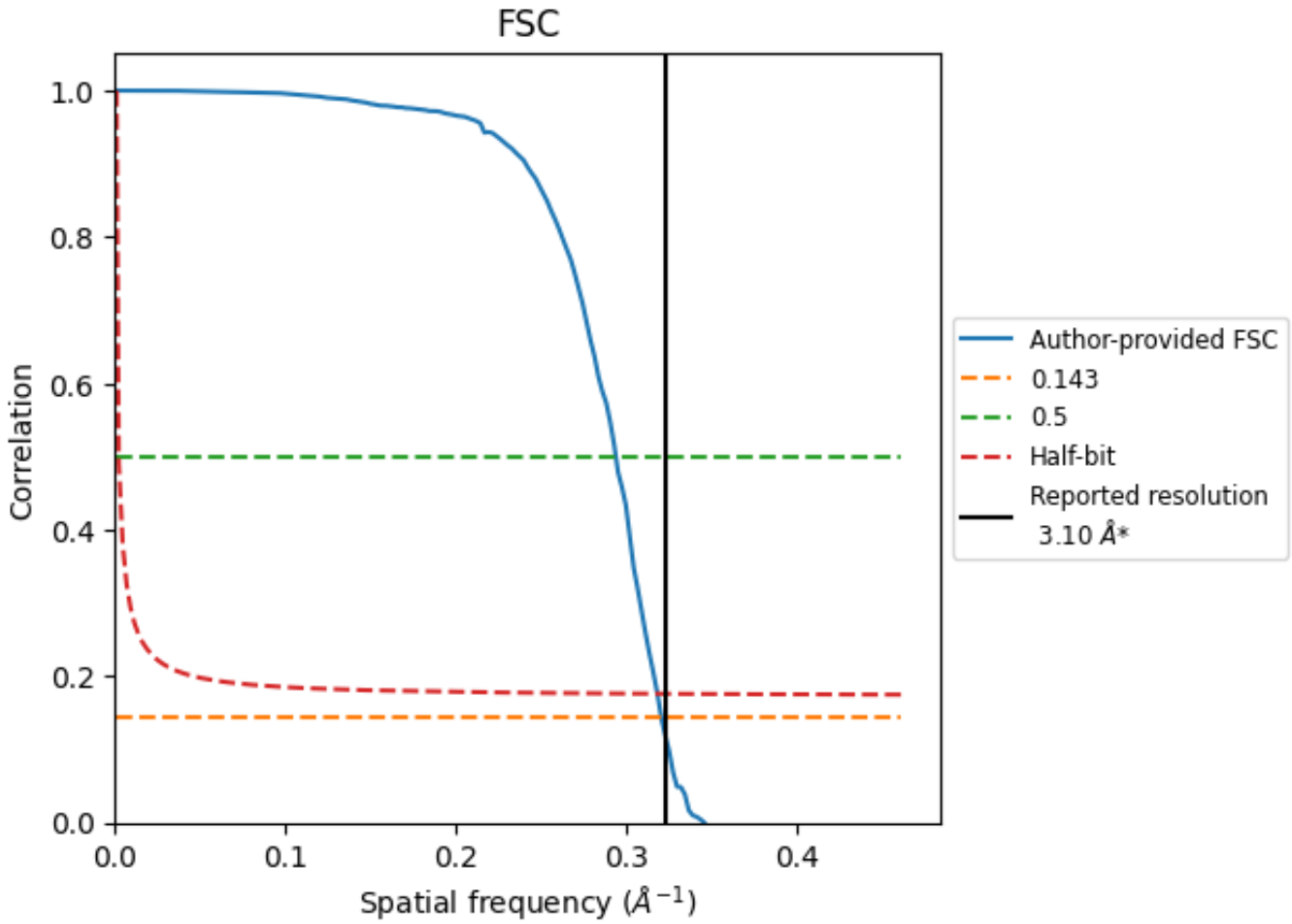


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

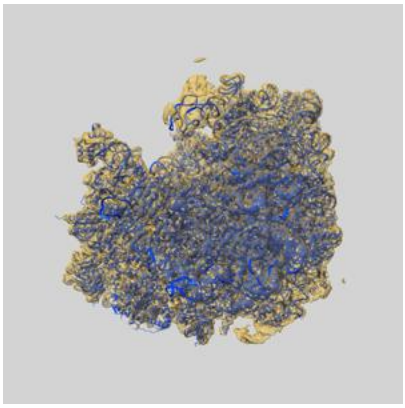
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.40	3.14
Unmasked-calculated*	-	-	-

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

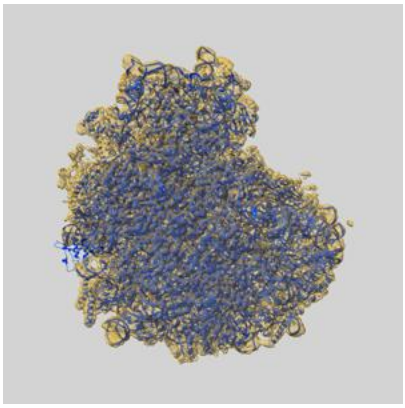
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4474 and PDB model 6Q8Y. Per-residue inclusion information can be found in section 3 on page 19.

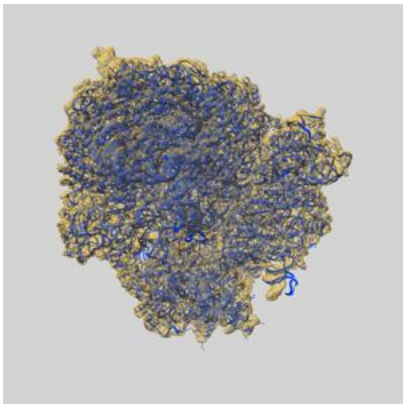
9.1 Map-model overlay



X



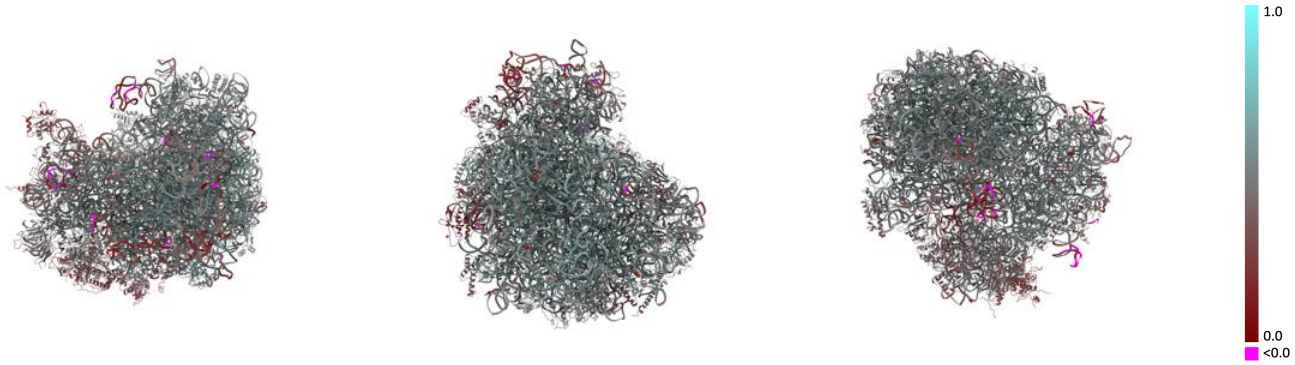
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

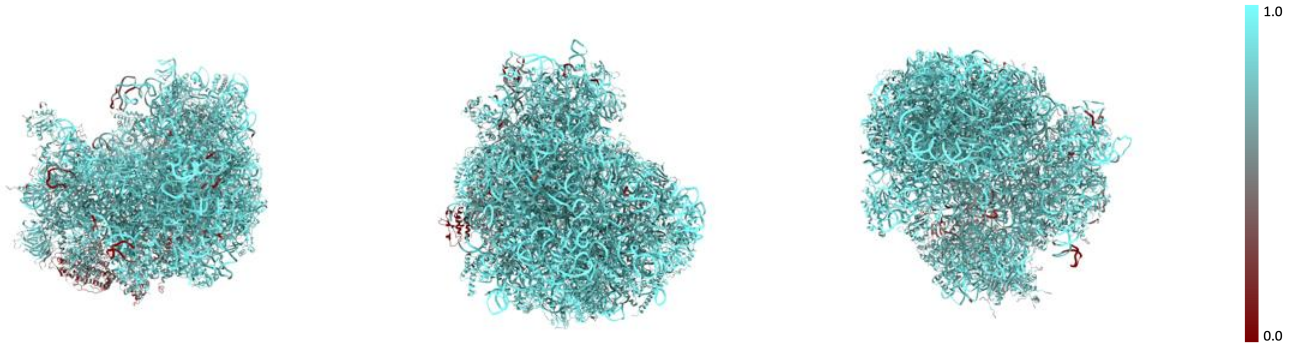
9.2 Q-score mapped to coordinate model



X Y Z

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

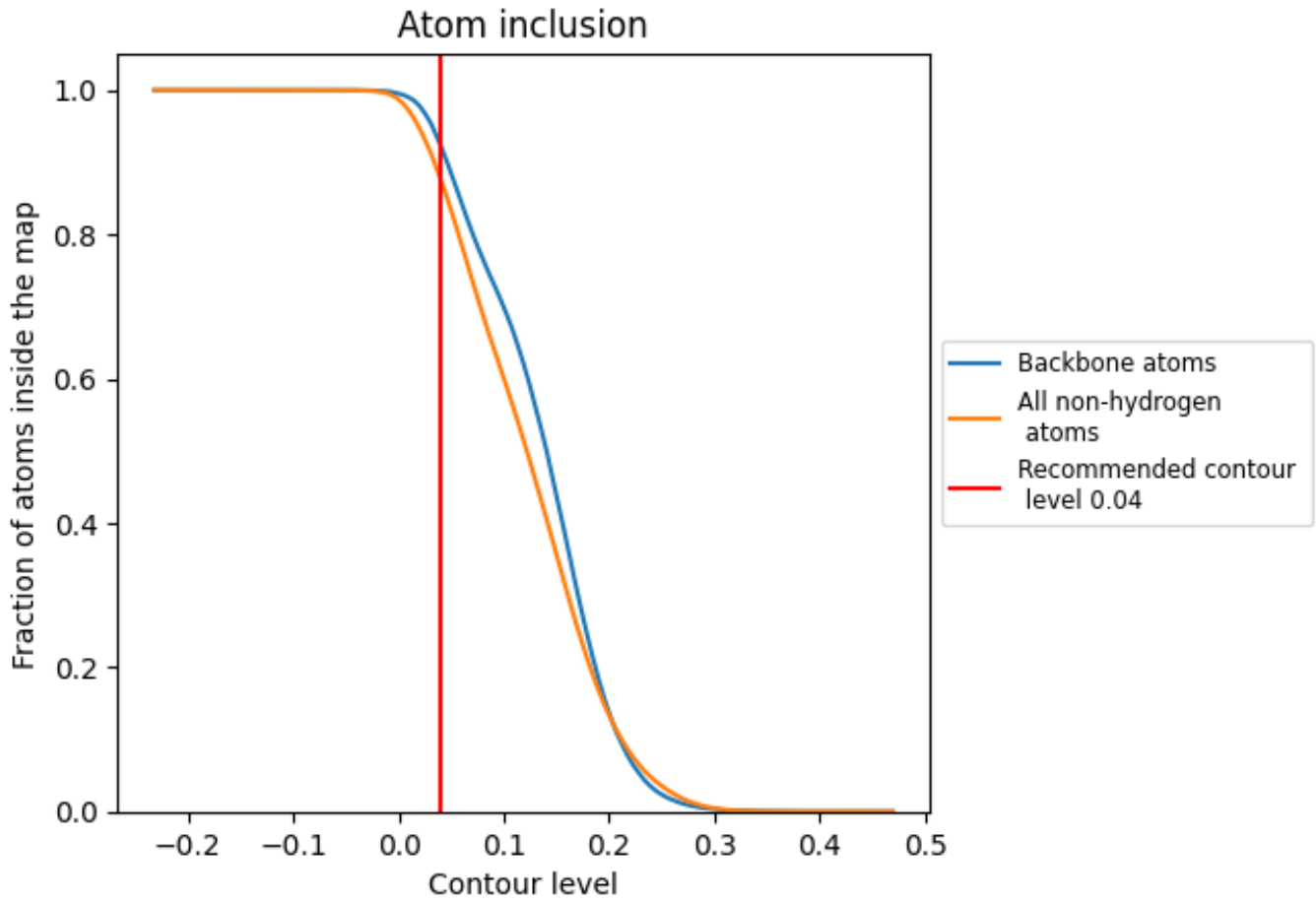
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8767	0.4840
2	0.9312	0.4700
A	0.8005	0.4360
AA	0.8544	0.4920
AB	0.8427	0.5260
AC	0.8456	0.4920
AD	0.8403	0.4890
AE	0.8330	0.5120
AF	0.8979	0.5580
AG	0.8160	0.4490
AH	0.8715	0.5240
AI	0.8097	0.4740
AJ	0.8722	0.5100
AK	0.8758	0.5100
AL	0.8723	0.5360
AM	0.8704	0.4830
AN	0.8758	0.5090
AO	0.8490	0.5030
AP	0.8335	0.5250
AQ	0.8766	0.5510
AR	0.8809	0.5320
AS	0.7925	0.5220
AT	0.8388	0.5320
AU	0.8666	0.5120
AV	0.8031	0.4750
AW	0.8749	0.5520
AX	0.8692	0.5180
AY	0.8644	0.5170
B	0.7715	0.4210
BA	0.8843	0.5280
BB	0.8824	0.5210
BC	0.8529	0.5110
BD	0.8041	0.4710
BE	0.8827	0.5210
BF	0.8232	0.4880

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Chain	Atom inclusion	Q-score
BG	0.8652	0.5330
BH	0.8516	0.5090
BI	0.8417	0.4480
BJ	0.8500	0.5060
BK	0.8867	0.5440
BL	0.8632	0.4760
BM	0.8615	0.4890
BN	0.8697	0.5320
BO	0.8743	0.5020
BP	0.8674	0.5070
BQ	0.9596	0.5200
BR	0.9822	0.4980
BS	0.9717	0.5500
C	0.7513	0.3850
D	0.6736	0.2640
E	0.7540	0.3870
F	0.8239	0.4640
G	0.7893	0.4330
H	0.7921	0.4120
I	0.8078	0.4130
J	0.7357	0.4070
K	0.8007	0.3730
L	0.7505	0.4470
M	0.8774	0.4910
N	0.7088	0.2760
O	0.7877	0.4260
P	0.8277	0.4600
Q	0.8231	0.4760
R	0.8313	0.4910
S	0.8351	0.4980
T	0.7898	0.4180
U	0.8132	0.4330
V	0.7848	0.4590
W	0.8125	0.4480
X	0.8113	0.5070
Y	0.8390	0.5020
Z	0.8817	0.5040
a	0.8358	0.4730
b	0.8697	0.5270
c	0.8272	0.5180
d	0.7743	0.4190
e	0.7595	0.4340

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Chain	Atom inclusion	Q-score
f	0.8453	0.4920
g	0.7834	0.4470
l	0.6685	0.3580
m	0.8194	0.3660
n	0.9081	0.4430
z	0.2308	0.2590