



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 08:20 pm BST

PDB ID : 7NRC / pdb\_00007nrc  
EMDB ID : EMD-12534  
Title : Structure of the yeast Gcn1 bound to a leading stalled 80S ribosome with Rbg2, Gir2, A- and P-tRNA and eIF5A  
Authors : Pochopien, A.A.; Beckert, B.; Wilson, D.N.  
Deposited on : 2021-03-03  
Resolution : 3.90 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](mailto: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>.

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

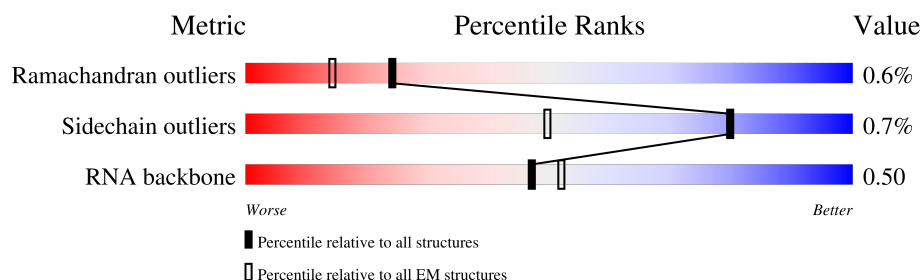
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 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 3.90 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S2	1800	
2	SI	6	
3	SP	206	
4	SQ	232	
5	SE	117	
6	SR	216	
7	SA	222	
8	SS	258	

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Mol	Chain	Length	Quality of chain
9	SB	206	 9% 99%
10	ST	228	 98%
11	SU	184	 14% 97%
12	SV	198	 94% 6%
13	SW	184	 8% 97%
14	SC	92	 10% 99%
15	SX	142	 99%
16	SD	121	 26% 97%
17	SY	150	 5% 98%
18	SZ	127	 98%
19	SF	141	 99%
20	SG	125	 10% 97%
21	SH	145	 7% 97%
22	SI	143	 9% 99%
23	SJ	100	 7% 99%
24	Sa	87	 99%
25	Sb	129	 98%
26	Sc	144	 99%
27	Sd	134	 99%
28	SK	82	 20% 98%
29	Se	97	 100%
30	Sf	81	 9% 98%
31	SM	53	 100%
32	Sg	57	 7% 100%
33	SN	73	 26% 96%

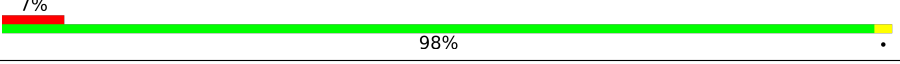
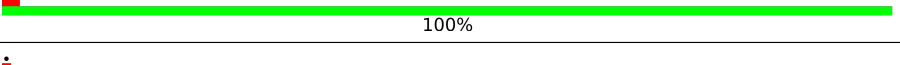
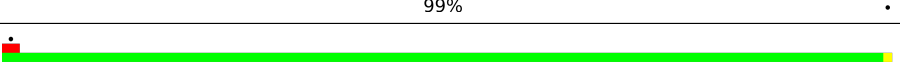
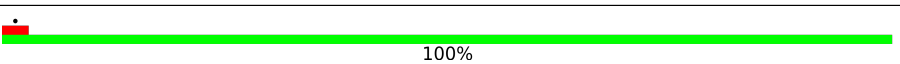
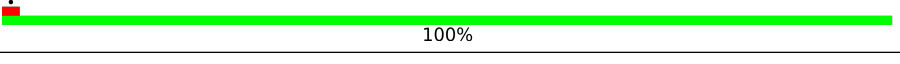
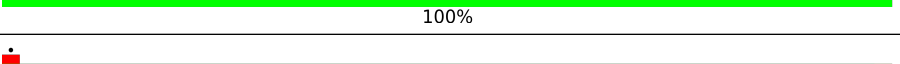
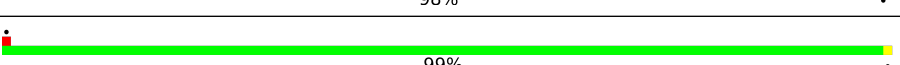
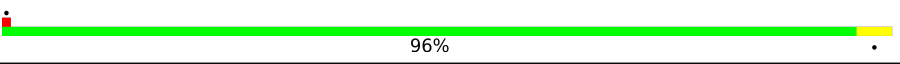
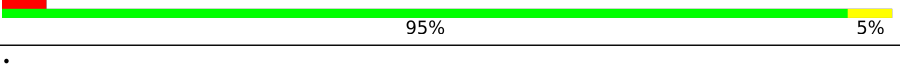
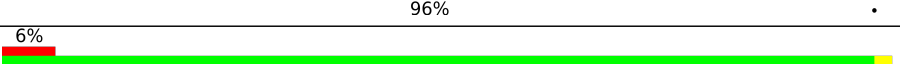
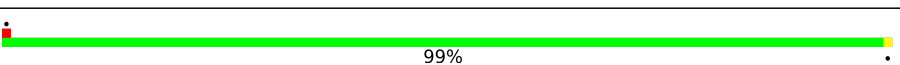
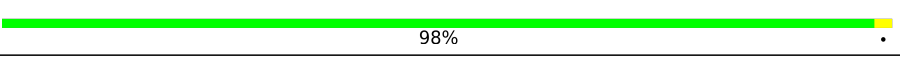
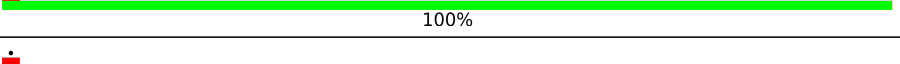
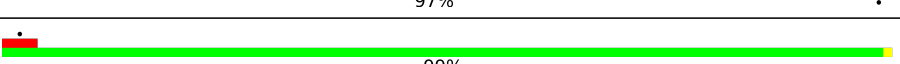
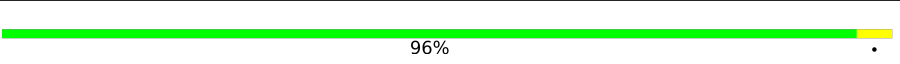
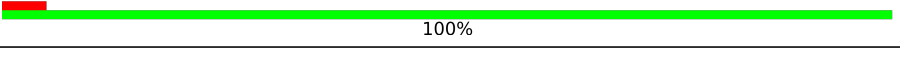
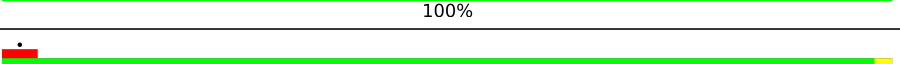
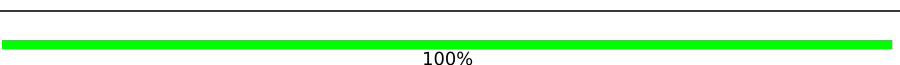
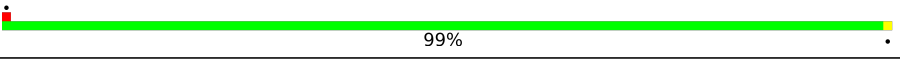
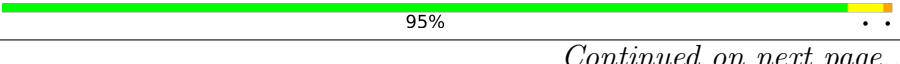



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Mol	Chain	Length	Quality of chain
34	SO	312	
35	SL	63	
36	Sm	76	
37	Sn	75	
38	So	366	
39	Sp	48	
40	LA	3394	
41	LB	121	
42	LC	158	
43	LD	251	
44	LE	386	
45	LF	361	
46	LG	294	
47	LH	175	
48	LI	222	
49	LJ	233	
50	LK	191	
51	LL	218	
52	LM	169	
53	LN	193	
54	LO	136	
55	LP	203	
56	LQ	197	
57	LR	183	
58	LS	185	

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Mol	Chain	Length	Quality of chain
59	LT	188	
60	LU	171	
61	LV	159	
62	LW	100	
63	LX	136	
64	LY	65	
65	LZ	121	
66	La	125	
67	Lb	135	
68	Lc	148	
69	Ld	58	
70	Le	96	
71	Lf	109	
72	Lg	127	
73	Lh	106	
74	Li	112	
75	Lj	119	
76	Lk	99	
77	Ll	81	
78	Lm	77	
79	Ln	50	
80	Lo	52	
81	Lp	25	
82	Lq	103	
83	Lr	91	

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Mol	Chain	Length	Quality of chain
84	Ls	154	
85	Lt	210	
86	A	1209	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	5CT	Ls	51	X	-	-	-

## 2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 213576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA (1771-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1771	Total	C	N	O	P	0	0
			37739	16872	6683	12413	1771		

- Molecule 2 is a RNA chain called RNA (5'-R(P\*AP\*UP\*GP\*AP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Sl	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 3 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SP	206	Total	C	N	O	S	0	0
			1603	1030	284	287	2		

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SQ	226	Total	C	N	O	S	0	0
			1798	1139	330	325	4		

- Molecule 5 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	117	Total	C	N	O	S	0	0
			916	583	171	155	7		

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SR	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SA	222	Total	C	N	O	S	0	0
			1729	1098	312	313	6		

- Molecule 8 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SS	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 9 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SB	206	Total	C	N	O	S	0	0
			1605	1005	299	298	3		

- Molecule 10 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	ST	228	Total	C	N	O	S	0	0
			1815	1138	351	323	3		

- Molecule 11 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SU	184	Total	C	N	O		0	0
			1473	946	263	264			

- Molecule 12 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SV	187	Total	C	N	O	S	0	0
			1476	916	295	263	2		

- Molecule 13 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SW	184	Total	C	N	O	S	0	0
			1479	935	285	258	1		

- Molecule 14 is a protein called 40S ribosomal protein S10-A.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	SC	92	Total	C	N	O	S	0	0
			752	487	122	141	2		

- Molecule 15 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SX	142	Total	C	N	O	S	0	0
			1142	733	217	189	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SD	121	Total	C	N	O	S	0	0
			875	551	153	169	2		

- Molecule 17 is a protein called 40S ribosomal protein S13.

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

- Molecule 18 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SZ	127	Total	C	N	O	S	0	0
			923	568	185	167	3		

- Molecule 19 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	SF	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 20 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SG	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 21 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SH	145	Total	C	N	O	S	0	0
			1188	741	237	208	2		

- Molecule 22 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SI	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 23 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SJ	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 24 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Sa	87	Total	C	N	O	S	0	0
			673	415	125	131	2		

- Molecule 25 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 26 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 27 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Sd	134	Total	C	N	O	0	0
			1032	651	195	186		

- Molecule 28 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	SK	82	Total	C	N	O		
			651	416	123	112	0	0

- Molecule 29 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Se	97	Total	C	N	O	S		
			765	473	160	127	5	0	0

- Molecule 30 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sg	57	Total	C	N	O	S		
			451	284	93	73	1	0	0

- Molecule 33 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SN	73	Total	C	N	O	S		
			556	352	105	95	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SN	97	ALA	LYS	variant	UNP P05759

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SO	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		

- Molecule 35 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SL	63	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 36 is a RNA chain called tRNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sm	76	Total	C	N	O	P	0	0
			1611	721	281	534	75		

- Molecule 37 is a RNA chain called tRNA (75-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Sn	75	Total	C	N	O	P	0	0
			1606	716	297	518	75		

- Molecule 38 is a protein called Ribosome-interacting GTPase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	So	347	Total	C	N	O	S	0	0
			2729	1723	478	518	10		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
So	62	ALA	LYS	variant	UNP P53295
So	92	ALA	ILE	variant	UNP P53295
So	94	GLU	HIS	variant	UNP P53295
So	96	GLU	ALA	variant	UNP P53295
So	134	LYS	ARG	variant	UNP P53295
So	271	ALA	THR	variant	UNP P53295
So	299	ALA	TYR	variant	UNP P53295
So	303	ALA	ARG	variant	UNP P53295
So	318	ASP	ASN	variant	UNP P53295
So	361	GLU	ASP	variant	UNP P53295

- Molecule 39 is a protein called GIR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	Sp	48	Total	C	N	O	0	0
			240	144	48	48		

- Molecule 40 is a RNA chain called 25S rRNA (3184-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LA	3184	Total	C	N	O	P	0	0
			68091	30415	12259	22233	3184		

- Molecule 41 is a RNA chain called 5S rRNA (121-MER).

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

- Molecule 42 is a RNA chain called 5.8S rRNA (158-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LC	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 43 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LD	251	Total	C	N	O	S	0	0
			1899	1182	385	331	1		

- Molecule 44 is a protein called 60S ribosomal protein L3.

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

- Molecule 45 is a protein called 60S ribosomal protein L4-A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LG	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 47 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LH	167	Total	C	N	O		0	0
			1307	843	234	230			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LH	120	LYS	ASN	variant	UNP P05739

- Molecule 48 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 49 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 50 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LK	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 51 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LL	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 52 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LM	169	Total	C	N	O	S	0	0
			1346	843	252	247	4		

- Molecule 53 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LN	193	Total	C	N	O	S	0	0
			1543	962	315	266			

- Molecule 54 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 55 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 56 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 57 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LR	183	Total	C	N	O	S	0	0
			1416	879	284	253			

- Molecule 58 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 59 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	LT	188	Total	C	N	O		
			1515	932	323	260	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LU	171	Total	C	N	O	S		
			1437	925	266	243	3	0	0

- Molecule 61 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LV	159	Total	C	N	O	S		
			1272	802	245	221	4	0	0

- Molecule 62 is a protein called 60S ribosomal protein L22-A.

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

- Molecule 63 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 64 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LY	65	Total	C	N	O	S		
			528	339	104	84	1	0	0

- Molecule 65 is a protein called 60S ribosomal protein L25.

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

- Molecule 66 is a protein called 60S ribosomal protein L26-A.



Mol	Chain	Residues	Atoms				AltConf	Trace
66	La	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 67 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	Lb	135	Total	C	N	O	0	0
			1080	701	199	180		

- Molecule 68 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Lc	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 69 is a protein called 60S ribosomal protein L29.

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

- Molecule 70 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Le	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 71 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 72 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Lg	127	Total	C	N	O	S	0	0
			1017	644	205	167	1		

- Molecule 73 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 74 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 75 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 76 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lk	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 77 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ll	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 78 is a protein called 60S ribosomal protein L38.

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

- Molecule 79 is a protein called 60S ribosomal protein L39.

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

- Molecule 80 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Lo	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 81 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Lp	25	Total	C	N	O	S	0	0
			229	139	62	27	1		

- Molecule 82 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Lq	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 83 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 84 is a protein called eiF5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Ls	154	Total	C	N	O	S	0	0
			1143	709	195	230	9		

- Molecule 85 is a protein called L1 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
85	Lt	210	Total	C	N	O	0	0
			1050	630	210	210		

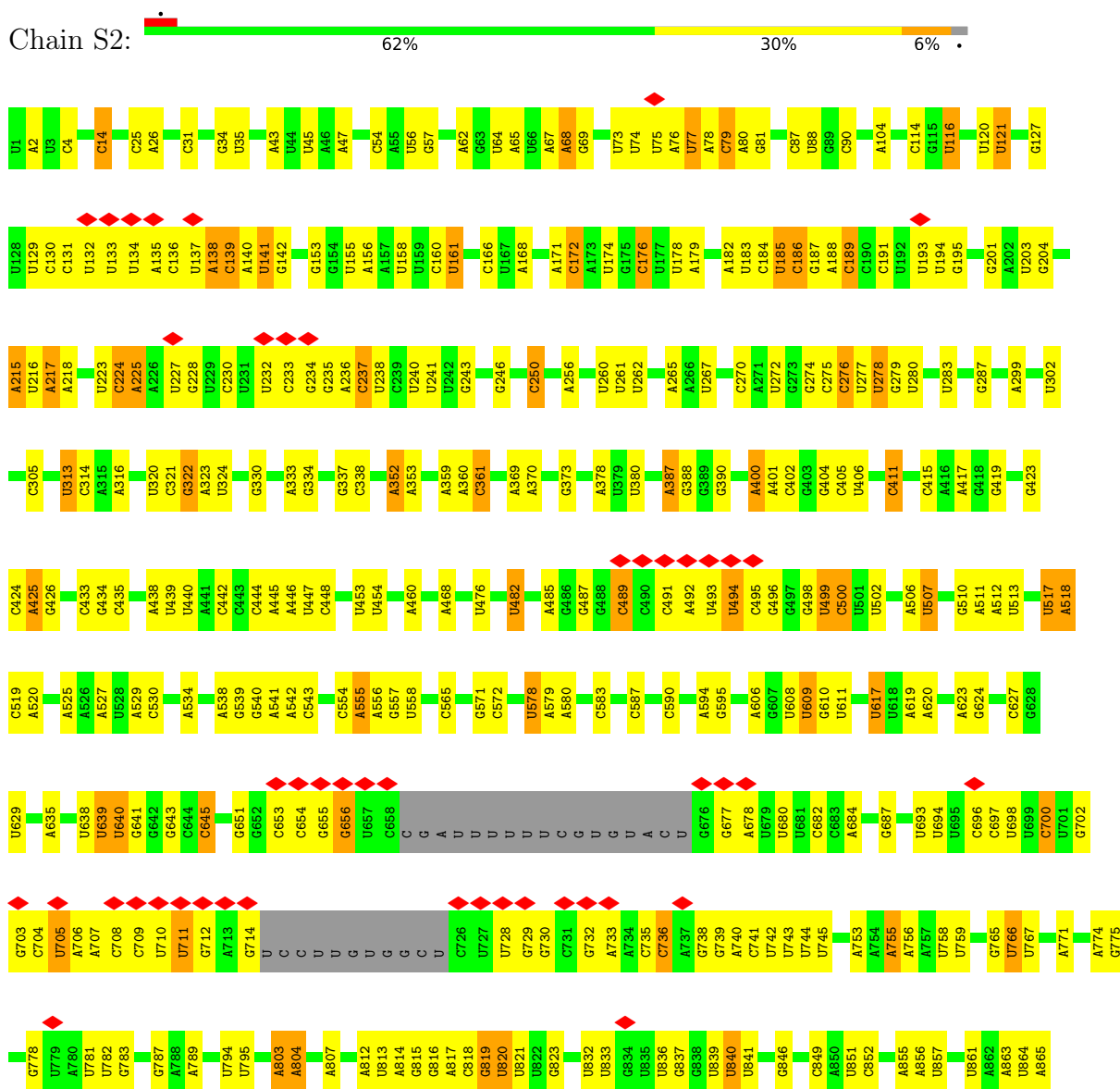
- Molecule 86 is a protein called GCN1.

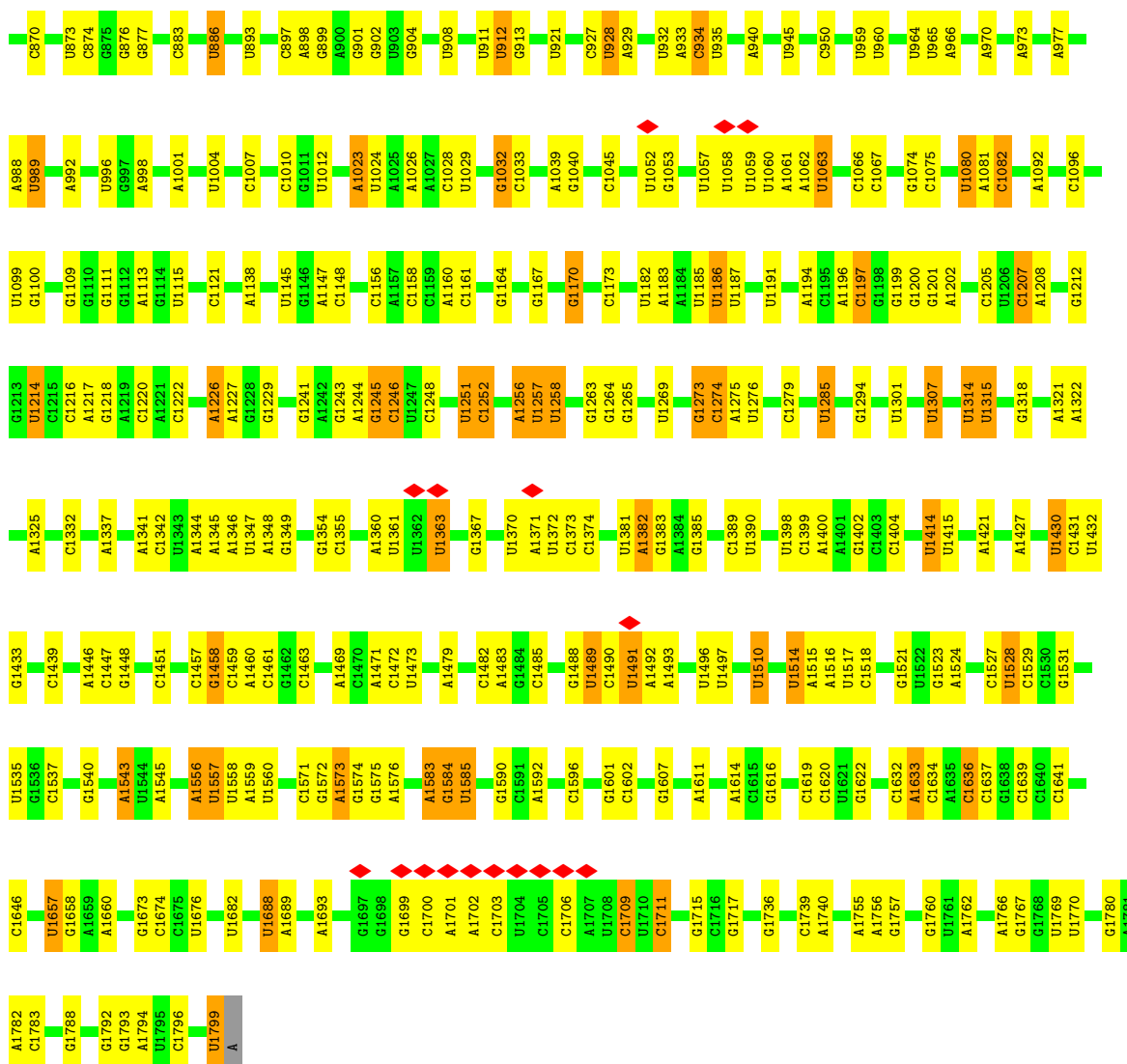
Mol	Chain	Residues	Atoms				AltConf	Trace
86	A	1209	Total	C	N	O	1	0
			6029	3609	1210	1210		

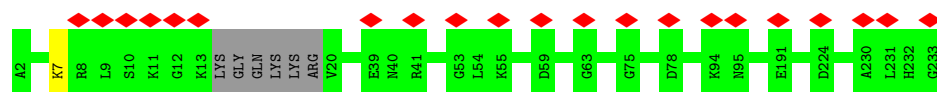
### 3 Residue-property plots

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

#### • Molecule 1: 18S rRNA (1771-MER)

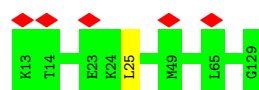






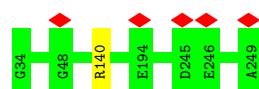
- Molecule 5: 40S ribosomal protein S15

Chain SE: 99%



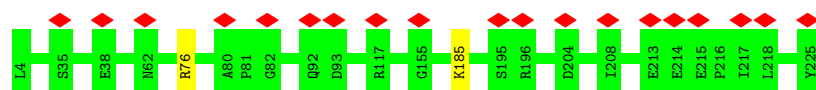
- Molecule 6: 40S ribosomal protein S2

Chain SR: 100%



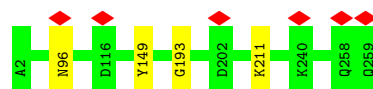
- Molecule 7: 40S ribosomal protein S3

Chain SA: 9% 99%



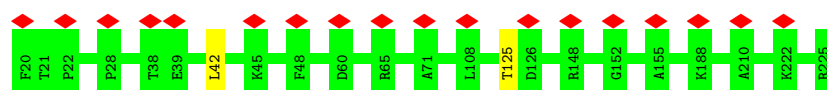
- Molecule 8: 40S ribosomal protein S4-A

Chain SS: 98%



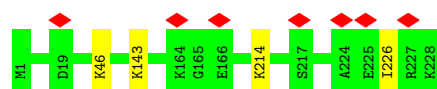
- Molecule 9: 40S ribosomal protein S5

Chain SB: 9% 99%

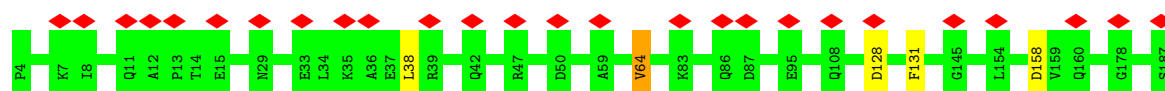


- Molecule 10: 40S ribosomal protein S6-A

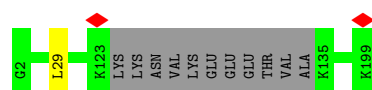
Chain ST: 98%



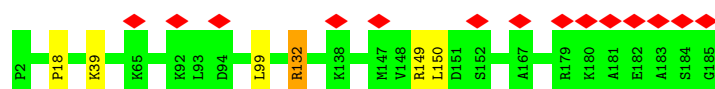
- Molecule 11: 40S ribosomal protein S7-A



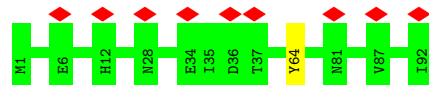
- Molecule 12: 40S ribosomal protein S8-A



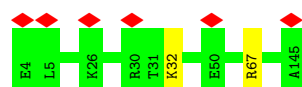
- Molecule 13: 40S ribosomal protein S9-A



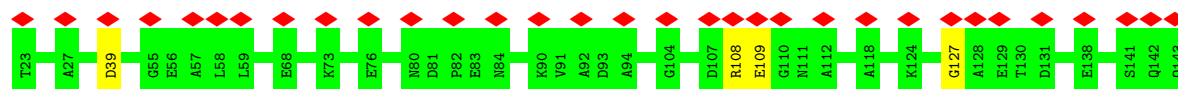
- Molecule 14: 40S ribosomal protein S10-A



- Molecule 15: 40S ribosomal protein S11-A



- Molecule 16: 40S ribosomal protein S12

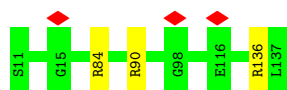


- Molecule 17: 40S ribosomal protein S13



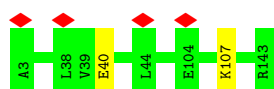
- Molecule 18: 40S ribosomal protein S14-B

Chain SZ:  98%



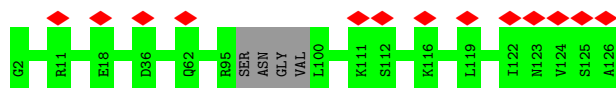
- Molecule 19: 40S ribosomal protein S16-A

Chain SF:  99%



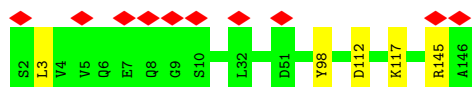
- Molecule 20: 40S ribosomal protein S17-B

Chain SG:  10% 97%



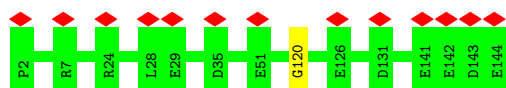
- Molecule 21: 40S ribosomal protein S18-A

Chain SH:  7% 97%



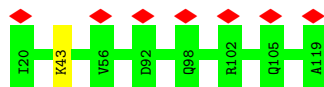
- Molecule 22: 40S ribosomal protein S19-A

Chain SI:  9% 99%



- Molecule 23: 40S ribosomal protein S20

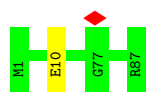
Chain SJ:  7% 99%



- Molecule 24: 40S ribosomal protein S21-A

Chain Sa:  99%





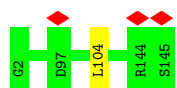
- Molecule 25: 40S ribosomal protein S22-A

Chain Sb: 98%



- Molecule 26: 40S ribosomal protein S23-A

Chain Sc: 99%



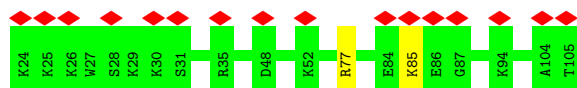
- Molecule 27: 40S ribosomal protein S24-A

Chain Sd: 99%



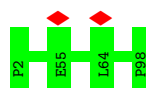
- Molecule 28: 40S ribosomal protein S25-A

Chain SK: 20% 98%



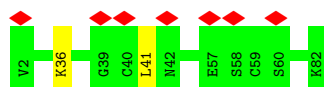
- Molecule 29: 40S ribosomal protein S26-B

Chain Se: 100%



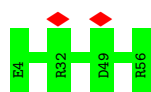
- Molecule 30: 40S ribosomal protein S27-A

Chain Sf: 9% 98%



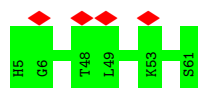
- Molecule 31: 40S ribosomal protein S29-A

Chain SM:  100%



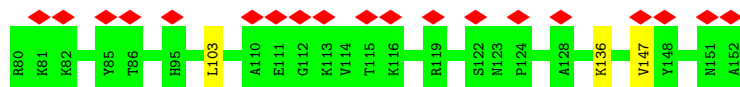
- Molecule 32: 40S ribosomal protein S30-A

Chain Sg:  7% 100%



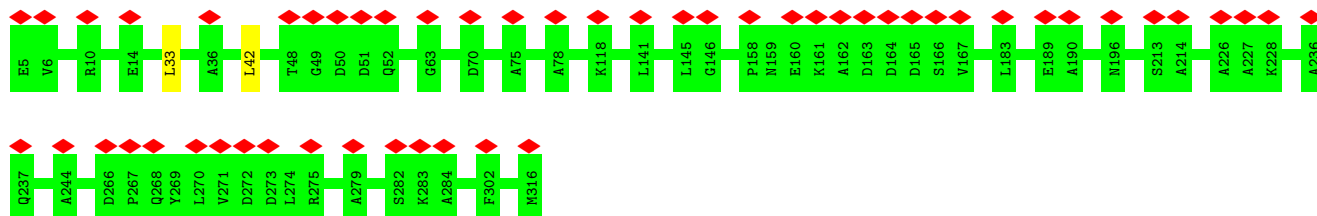
- Molecule 33: 40S ribosomal protein S31

Chain SN:  26% 96%



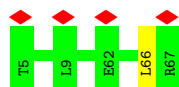
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SO:  17% 99%



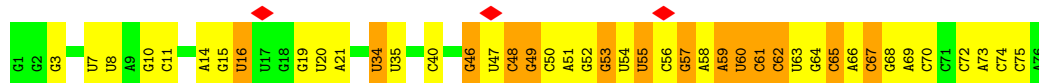
- Molecule 35: 40S ribosomal protein S28-A

Chain SL:  6% 98%

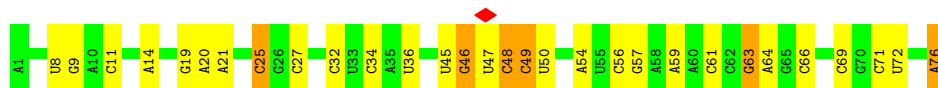


- Molecule 36: tRNA (76-MER)

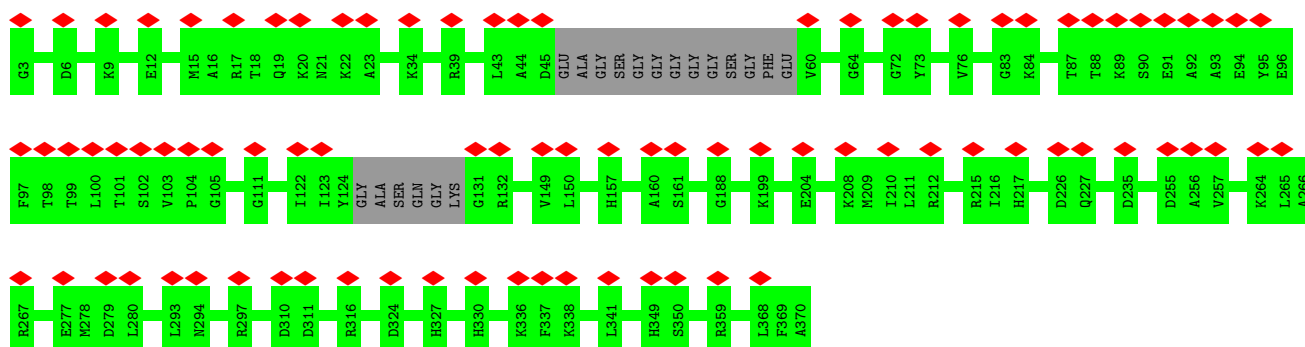
Chain Sm:  43% 38% 18%



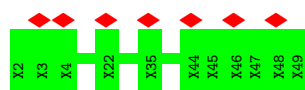
- Molecule 37: tRNA (75-MER)



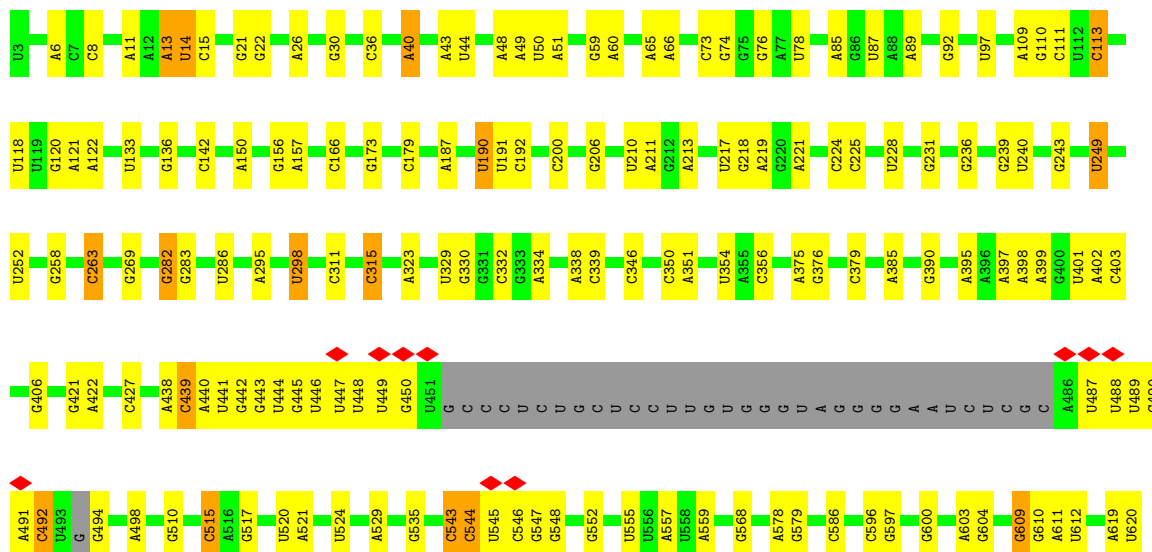
• Molecule 38: Ribosome-interacting GTPase 2



• Molecule 39: GIR2



• Molecule 40: 25S rRNA (3184-MER)

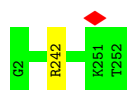






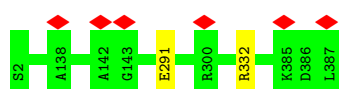
- Molecule 43: 60S ribosomal protein L2-A

Chain LD:  100%



- Molecule 44: 60S ribosomal protein L3

Chain LE:  99%



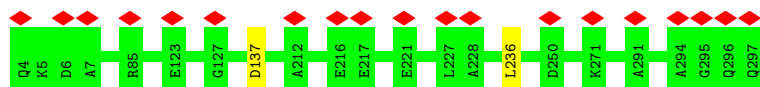
- Molecule 45: 60S ribosomal protein L4-A

Chain LF:  99%



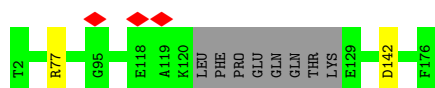
- Molecule 46: 60S ribosomal protein L5

Chain LG:  6%  99%



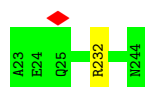
- Molecule 47: 60S ribosomal protein L6-B

Chain LH:  94%  5%



- Molecule 48: 60S ribosomal protein L7-A

Chain LI:  100%



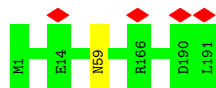
- Molecule 49: 60S ribosomal protein L8-A

Chain LJ:  98%



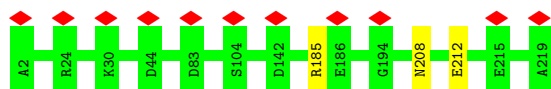
- Molecule 50: 60S ribosomal protein L9-A

Chain LK: 99%



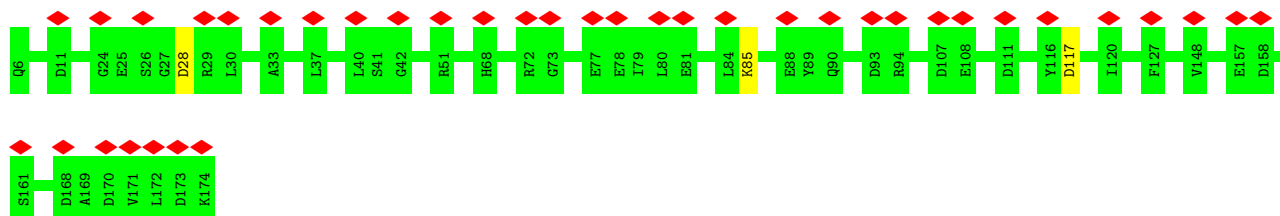
- Molecule 51: 60S ribosomal protein L10

Chain LL: 5% 99%



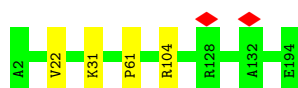
- Molecule 52: 60S ribosomal protein L11-B

Chain LM: 22% 98%



- Molecule 53: 60S ribosomal protein L13-A

Chain LN: 98%



- Molecule 54: 60S ribosomal protein L14-A

Chain LO: 100%

There are no outlier residues recorded for this chain.

- Molecule 55: 60S ribosomal protein L15-A

Chain LP: 99%



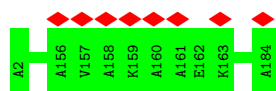
- Molecule 56: 60S ribosomal protein L16-A

Chain LQ:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: 60S ribosomal protein L17-A

Chain LR:  100%



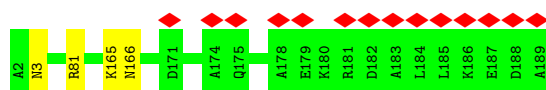
- Molecule 58: 60S ribosomal protein L18-A

Chain LS:  97%



- Molecule 59: 60S ribosomal protein L19-A

Chain LT:  98%



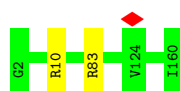
- Molecule 60: 60S ribosomal protein L20-A

Chain LU:  100%



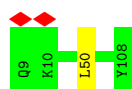
- Molecule 61: 60S ribosomal protein L21-A

Chain LV:  99%



- Molecule 62: 60S ribosomal protein L22-A

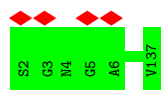
Chain LW:  99%





- Molecule 63: 60S ribosomal protein L23-A

Chain LX:  100%



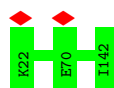
- Molecule 64: 60S ribosomal protein L24-A

Chain LY:  100%



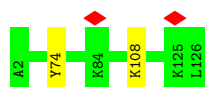
- Molecule 65: 60S ribosomal protein L25

Chain LZ:  100%



- Molecule 66: 60S ribosomal protein L26-A

Chain La:  98%



- Molecule 67: 60S ribosomal protein L27-A

Chain Lb:  99%



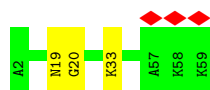
- Molecule 68: 60S ribosomal protein L28

Chain Lc:  96%



- Molecule 69: 60S ribosomal protein L29

Chain Ld:  95%



- Molecule 70: 60S ribosomal protein L30

Chain Le: 96%



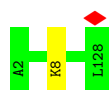
- Molecule 71: 60S ribosomal protein L31-A

Chain Lf: 98%



- Molecule 72: 60S ribosomal protein L32

Chain Lg: 99%



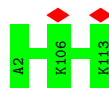
- Molecule 73: 60S ribosomal protein L33-A

Chain Lh: 98%



- Molecule 74: 60S ribosomal protein L34-A

Chain Li: 100%



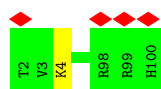
- Molecule 75: 60S ribosomal protein L35-A

Chain Lj: 97%



- Molecule 76: 60S ribosomal protein L36-A

Chain Lk:  99%



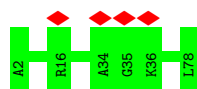
- Molecule 77: 60S ribosomal protein L37-A

Chain Ll:  96%



- Molecule 78: 60S ribosomal protein L38

Chain Lm:  100%



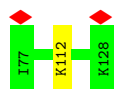
- Molecule 79: 60S ribosomal protein L39

Chain Ln:  100%

There are no outlier residues recorded for this chain.

- Molecule 80: 60S ribosomal protein L40-A

Chain Lo:  98%



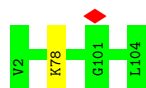
- Molecule 81: 60S ribosomal protein L41-A

Chain Lp:  100%

There are no outlier residues recorded for this chain.

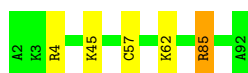
- Molecule 82: 60S ribosomal protein L42-A

Chain Lq:  99%

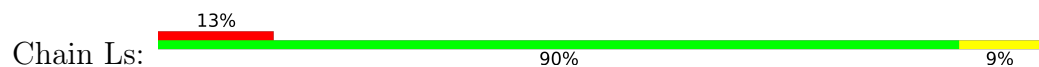


- Molecule 83: 60S ribosomal protein L43-A

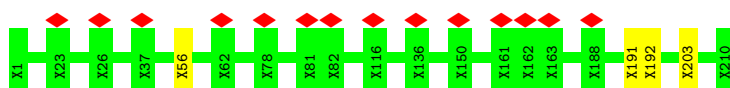
Chain Lr:  95%



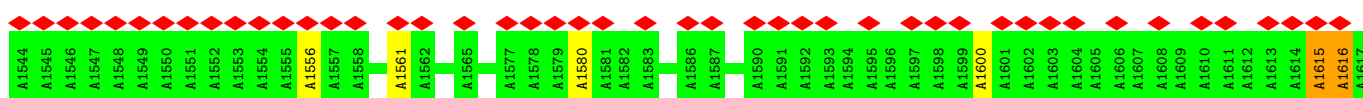
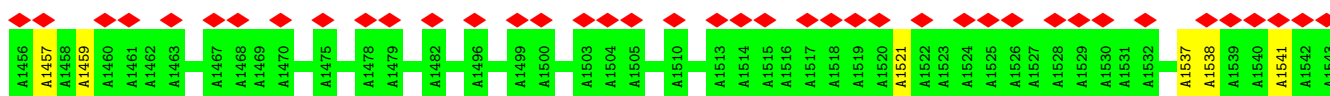
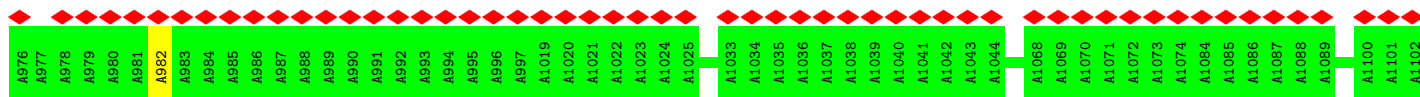
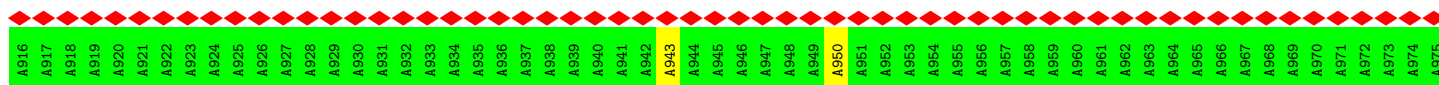
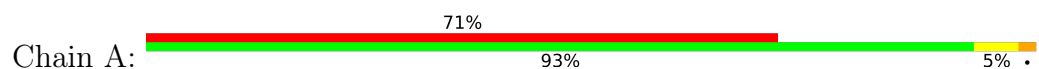
• Molecule 84: eiF5A



• Molecule 85: L1 60S ribosomal protein



• Molecule 86: GCN1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30016	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	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	0.512	Depositor
Minimum map value	-0.389	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	758.8, 758.8, 758.8	wwPDB
Map dimensions	700, 700, 700	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: 5CT

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	S2	0.46	0/42211	1.27	410/65773 (0.6%)
2	SI	0.52	0/147	1.18	0/227
3	SP	0.37	0/1644	0.74	1/2249 (0.0%)
4	SQ	0.37	0/1823	0.84	0/2447
5	SE	0.37	0/936	0.80	1/1259 (0.1%)
6	SR	0.40	0/1656	0.81	2/2251 (0.1%)
7	SA	0.36	0/1754	0.76	0/2361
8	SS	0.39	0/2097	0.84	2/2823 (0.1%)
9	SB	0.36	0/1625	0.73	0/2197
10	ST	0.38	0/1839	0.78	0/2460
11	SU	0.40	0/1498	0.86	5/2019 (0.2%)
12	SV	0.35	0/1501	0.75	1/2006 (0.0%)
13	SW	0.33	0/1504	0.76	3/2016 (0.1%)
14	SC	0.37	0/769	0.78	0/1039
15	SX	0.34	0/1168	0.73	0/1575
16	SD	0.39	0/883	0.87	1/1199 (0.1%)
17	SY	0.38	0/1215	0.78	2/1638 (0.1%)
18	SZ	0.37	0/934	0.82	2/1257 (0.2%)
19	SF	0.37	0/1125	0.79	0/1510
20	SG	0.34	0/957	0.74	0/1283
21	SH	0.36	0/1207	0.80	3/1623 (0.2%)
22	SI	0.39	0/1130	0.76	0/1517
23	SJ	0.35	0/807	0.77	0/1091
24	Sa	0.33	0/682	0.75	1/921 (0.1%)
25	Sb	0.39	0/1038	0.83	2/1395 (0.1%)
26	Sc	0.39	0/1139	0.78	1/1518 (0.1%)
27	Sd	0.38	0/1046	0.79	2/1401 (0.1%)
28	SK	0.39	0/661	0.89	2/888 (0.2%)
29	Se	0.35	0/778	0.74	0/1042
30	Sf	0.31	0/620	0.80	1/838 (0.1%)
31	SM	0.39	0/452	0.79	0/600
32	Sg	0.32	0/459	0.80	0/611

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	SN	0.37	0/567	0.85	2/764 (0.3%)
34	SO	0.34	0/2436	0.83	2/3318 (0.1%)
35	SL	0.39	0/493	0.95	1/663 (0.2%)
36	Sm	0.49	0/1799	1.53	43/2801 (1.5%)
37	Sn	0.46	0/1796	1.37	24/2799 (0.9%)
38	So	0.29	0/2769	0.57	0/3736
40	LA	0.47	1/76214 (0.0%)	1.20	582/118821 (0.5%)
41	LB	0.39	0/2883	1.15	20/4491 (0.4%)
42	LC	0.45	0/3746	1.19	25/5832 (0.4%)
43	LD	0.36	0/1933	0.76	0/2598
44	LE	0.38	0/3146	0.74	1/4228 (0.0%)
45	LF	0.36	0/2800	0.73	0/3790
46	LG	0.37	0/2400	0.74	2/3239 (0.1%)
47	LH	0.37	0/1329	0.76	2/1794 (0.1%)
48	LI	0.38	0/1821	0.68	0/2451
49	LJ	0.37	0/1836	0.72	0/2481
50	LK	0.36	0/1529	0.74	0/2060
51	LL	0.35	0/1801	0.73	1/2416 (0.0%)
52	LM	0.36	0/1367	0.80	2/1834 (0.1%)
53	LN	0.36	0/1568	0.71	1/2106 (0.0%)
54	LO	0.35	0/1068	0.69	0/1438
55	LP	0.44	0/1757	0.75	1/2354 (0.0%)
56	LQ	0.39	0/1585	0.69	0/2128
57	LR	0.37	0/1439	0.69	0/1938
58	LS	0.35	0/1465	0.72	1/1965 (0.1%)
59	LT	0.34	0/1532	0.65	0/2043
60	LU	0.36	0/1473	0.69	0/1980
61	LV	0.35	0/1296	0.71	0/1739
62	LW	0.37	0/812	0.73	1/1099 (0.1%)
63	LX	0.34	0/1018	0.74	0/1369
64	LY	0.31	0/540	0.56	0/717
65	LZ	0.36	0/979	0.74	0/1321
66	La	0.31	0/995	0.68	0/1329
67	Lb	0.33	0/1106	0.68	0/1485
68	Lc	0.36	0/1200	0.74	2/1607 (0.1%)
69	Ld	0.33	0/473	0.69	0/629
70	Le	0.36	0/745	0.76	1/1001 (0.1%)
71	Lf	0.36	0/890	0.75	0/1196
72	Lg	0.33	0/1038	0.69	0/1390
73	Lh	0.37	0/868	0.81	1/1168 (0.1%)
74	Li	0.40	0/890	0.72	0/1189
75	Lj	0.32	0/978	0.70	1/1301 (0.1%)
76	Lk	0.34	0/772	0.69	0/1026



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
77	Ll	0.45	0/660	0.81	0/875
78	Lm	0.36	0/618	0.77	0/826
79	Ln	0.34	0/443	0.74	0/588
80	Lo	0.33	0/416	0.72	0/553
81	Lp	0.37	0/230	0.74	0/296
82	Lq	0.37	0/836	0.76	0/1104
83	Lr	0.38	0/701	0.72	1/934 (0.1%)
84	Ls	0.39	0/1142	0.99	10/1537 (0.7%)
86	A	0.92	21/6015 (0.3%)	0.89	19/8386 (0.2%)
All	All	0.45	22/227518 (0.0%)	1.07	1188/333767 (0.4%)

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
8	SS	0	1
9	SB	0	2
11	SU	0	1
16	SD	0	1
18	SZ	0	1
19	SF	0	1
22	SI	0	1
25	Sb	0	1
33	SN	0	1
45	LF	0	3
48	LI	0	1
49	LJ	0	3
58	LS	0	1
68	Lc	0	2
69	Ld	0	2
70	Le	0	1
71	Lf	0	1
75	Lj	0	1
84	Ls	1	2
85	Lt	0	4
86	A	0	12
All	All	1	43

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	A	1361	PRO	N-CA	13.63	1.70	1.47
86	A	1421	PRO	N-CA	13.12	1.69	1.47
86	A	1223	PRO	N-CA	13.01	1.69	1.47
86	A	2351	ALA	N-CA	12.07	1.70	1.46
86	A	1840	ALA	N-CA	12.04	1.70	1.46
86	A	2040	ALA	N-CA	12.04	1.70	1.46
86	A	2240	ALA	N-CA	12.02	1.70	1.46
86	A	2300	ALA	N-CA	11.66	1.69	1.46
86	A	2411	ALA	N-CA	11.65	1.69	1.46
86	A	1900	ALA	N-CA	11.61	1.69	1.46
86	A	1181	GLU	C-N	7.98	1.49	1.34
86	A	1360	GLY	C-N	6.08	1.45	1.34
86	A	1420	VAL	C-N	6.02	1.45	1.34
86	A	1616	ALA	C-O	5.92	1.34	1.23
86	A	2239	ALA	C-N	5.17	1.46	1.34
86	A	2350	ALA	C-N	5.15	1.45	1.34
86	A	2039	ALA	C-N	5.14	1.45	1.34
86	A	1839	ALA	C-N	5.13	1.45	1.34
86	A	2410	ALA	C-N	5.05	1.45	1.34
86	A	2299	ALA	C-N	5.04	1.45	1.34
86	A	1899	ALA	C-N	5.03	1.45	1.34
40	LA	1263	A	N9-C4	5.02	1.40	1.37

All (1188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	3217	C	N1-C2-O2	13.82	127.19	118.90
37	Sn	49	C	C6-N1-C2	-12.90	115.14	120.30
40	LA	2492	C	N1-C2-O2	12.72	126.53	118.90
86	A	1340	LYS	O-C-N	-12.26	103.08	122.70
86	A	2019	ALA	O-C-N	-12.22	103.15	122.70
86	A	1819	ALA	O-C-N	-12.20	103.18	122.70
86	A	2330	ALA	O-C-N	-12.18	103.21	122.70
40	LA	2492	C	C2-N1-C1'	12.05	132.05	118.80
40	LA	3217	C	C2-N1-C1'	11.95	131.95	118.80
1	S2	934	C	C2-N1-C1'	11.85	131.84	118.80
37	Sn	48	C	C6-N1-C2	-11.84	115.56	120.30
42	LC	125	U	C2-N1-C1'	11.54	131.55	117.70
42	LC	125	U	N1-C2-O2	11.23	130.66	122.80
1	S2	186	C	C2-N1-C1'	10.89	130.78	118.80
1	S2	276	C	N3-C2-O2	-10.82	114.33	121.90
40	LA	14	U	O5'-P-OP2	-10.78	96.00	105.70
40	LA	3217	C	N3-C2-O2	-10.70	114.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	1283	C	N3-C2-O2	-10.43	114.60	121.90
1	S2	934	C	N1-C2-O2	10.36	125.12	118.90
40	LA	1795	U	O5'-P-OP1	-10.31	96.42	105.70
40	LA	1283	C	N1-C2-O2	10.24	125.04	118.90
1	S2	1257	U	N3-C2-O2	-10.23	115.03	122.20
42	LC	125	U	N3-C2-O2	-10.21	115.05	122.20
8	SS	149	TYR	CB-CG-CD1	10.21	127.12	121.00
1	S2	736	C	N3-C2-O2	-10.19	114.77	121.90
37	Sn	49	C	C5-C6-N1	9.96	125.98	121.00
1	S2	1389	C	C2-N1-C1'	9.93	129.73	118.80
40	LA	2492	C	N3-C2-O2	-9.88	114.99	121.90
40	LA	3194	C	N3-C2-O2	-9.81	115.03	121.90
40	LA	2531	C	N1-C2-O2	9.66	124.70	118.90
40	LA	1280	C	N3-C2-O2	-9.65	115.15	121.90
36	Sm	62	C	C6-N1-C2	-9.62	116.45	120.30
36	Sm	60	U	N3-C2-O2	-9.55	115.52	122.20
40	LA	3181	C	N1-C2-O2	9.54	124.63	118.90
40	LA	2257	C	N1-C2-O2	9.53	124.62	118.90
36	Sm	60	U	N1-C2-O2	9.47	129.43	122.80
40	LA	2434	U	N3-C2-O2	-9.46	115.58	122.20
1	S2	1706	C	N3-C2-O2	-9.45	115.28	121.90
8	SS	149	TYR	CB-CG-CD2	-9.42	115.35	121.00
37	Sn	48	C	N1-C2-O2	9.38	124.53	118.90
40	LA	2531	C	C6-N1-C2	-9.31	116.58	120.30
37	Sn	48	C	N3-C2-O2	-9.25	115.42	121.90
1	S2	1799	U	N1-C2-O2	9.21	129.25	122.80
1	S2	1799	U	N3-C2-O2	-9.18	115.78	122.20
40	LA	2257	C	C2-N1-C1'	9.11	128.82	118.80
36	Sm	60	U	C2-N1-C1'	9.11	128.62	117.70
40	LA	2434	U	N1-C2-O2	9.08	129.16	122.80
1	S2	160	C	N1-C2-O2	9.05	124.33	118.90
40	LA	596	C	C6-N1-C2	-8.96	116.72	120.30
1	S2	861	U	C2-N1-C1'	8.94	128.42	117.70
36	Sm	62	C	N3-C2-O2	-8.90	115.67	121.90
40	LA	2366	C	C6-N1-C2	-8.89	116.74	120.30
1	S2	965	U	C2-N1-C1'	8.87	128.34	117.70
1	S2	874	C	C6-N1-C2	-8.86	116.76	120.30
1	S2	1257	U	N1-C2-O2	8.82	128.98	122.80
1	S2	1527	C	N1-C2-O2	8.81	124.19	118.90
40	LA	544	C	N3-C2-O2	-8.80	115.74	121.90
40	LA	922	U	C2-N1-C1'	8.77	128.22	117.70
40	LA	2526	C	C5-C6-N1	8.73	125.37	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1389	C	N1-C2-O2	8.65	124.09	118.90
40	LA	1227	C	N1-C2-O2	8.64	124.08	118.90
40	LA	1563	C	C6-N1-C2	-8.64	116.84	120.30
40	LA	2541	U	P-O3'-C3'	8.63	130.06	119.70
40	LA	3194	C	C6-N1-C2	-8.63	116.85	120.30
1	S2	160	C	N3-C2-O2	-8.60	115.88	121.90
42	LC	127	U	N1-C2-O2	8.58	128.80	122.80
1	S2	934	C	C6-N1-C1'	-8.57	110.51	120.80
1	S2	507	U	C5-C6-N1	8.56	126.98	122.70
40	LA	1579	C	N3-C2-O2	-8.55	115.91	121.90
40	LA	3181	C	C2-N1-C1'	8.55	128.20	118.80
40	LA	2492	C	C6-N1-C1'	-8.54	110.56	120.80
40	LA	2928	C	C6-N1-C2	-8.51	116.90	120.30
40	LA	1269	U	C2-N1-C1'	8.44	127.82	117.70
1	S2	225	A	N7-C8-N9	8.42	118.01	113.80
1	S2	767	U	N3-C2-O2	-8.41	116.31	122.20
1	S2	79	C	C6-N1-C2	-8.39	116.95	120.30
40	LA	1349	G	N3-C4-C5	-8.38	124.41	128.60
1	S2	1560	U	C2-N1-C1'	8.38	127.75	117.70
1	S2	656	G	C4-N9-C1'	8.35	137.36	126.50
40	LA	3217	C	C6-N1-C1'	-8.33	110.80	120.80
42	LC	127	U	C2-N1-C1'	8.33	127.69	117.70
1	S2	1458	G	C4-N9-C1'	8.32	137.32	126.50
41	LB	39	C	N1-C2-O2	8.31	123.89	118.90
1	S2	400	A	P-O3'-C3'	8.29	129.65	119.70
40	LA	2928	C	C5-C6-N1	8.26	125.13	121.00
1	S2	736	C	N1-C2-O2	8.25	123.85	118.90
40	LA	969	C	N1-C2-O2	8.24	123.84	118.90
40	LA	3317	U	N1-C2-O2	8.23	128.56	122.80
40	LA	3317	U	N3-C2-O2	-8.15	116.49	122.20
40	LA	2836	C	C2-N1-C1'	8.14	127.75	118.80
37	Sn	48	C	C5-C6-N1	8.12	125.06	121.00
40	LA	890	C	C6-N1-C2	-8.11	117.06	120.30
1	S2	1560	U	N3-C2-O2	-8.11	116.52	122.20
40	LA	3306	U	C2-N1-C1'	8.10	127.42	117.70
40	LA	1563	C	C5-C6-N1	8.09	125.05	121.00
1	S2	1082	C	C2-N1-C1'	8.08	127.69	118.80
40	LA	544	C	C6-N1-C2	-8.07	117.07	120.30
40	LA	1582	C	P-O3'-C3'	8.07	129.38	119.70
1	S2	1706	C	N1-C2-O2	8.06	123.74	118.90
40	LA	2366	C	C5-C6-N1	8.04	125.02	121.00
1	S2	1145	U	N3-C2-O2	-8.03	116.58	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	186	C	C6-N1-C1'	-7.99	111.21	120.80
40	LA	2531	C	N3-C2-O2	-7.96	116.33	121.90
1	S2	116	U	N3-C2-O2	-7.96	116.63	122.20
1	S2	1527	C	C2-N1-C1'	7.94	127.54	118.80
40	LA	1349	G	N3-C4-N9	7.93	130.76	126.00
40	LA	1496	C	C2-N1-C1'	7.92	127.51	118.80
1	S2	934	C	N3-C2-O2	-7.92	116.36	121.90
40	LA	2772	C	C2-N1-C1'	7.89	127.48	118.80
40	LA	2526	C	C6-N1-C2	-7.89	117.14	120.30
40	LA	1907	C	N1-C2-O2	7.89	123.63	118.90
1	S2	517	U	N3-C2-O2	-7.88	116.69	122.20
1	S2	965	U	N1-C2-O2	7.88	128.31	122.80
40	LA	444	U	N3-C2-O2	-7.87	116.69	122.20
1	S2	500	C	N3-C2-O2	-7.87	116.39	121.90
42	LC	127	U	N3-C2-O2	-7.86	116.70	122.20
40	LA	2405	C	C6-N1-C2	-7.83	117.17	120.30
1	S2	1145	U	N1-C2-O2	7.82	128.27	122.80
40	LA	2389	C	C6-N1-C2	-7.81	117.18	120.30
40	LA	2495	C	N1-C2-O2	7.81	123.59	118.90
40	LA	2112	U	OP2-P-O3'	7.80	122.36	105.20
1	S2	1023	A	OP2-P-O3'	7.79	122.35	105.20
40	LA	2873	U	C2-N1-C1'	7.79	127.05	117.70
84	Ls	120	LEU	CA-CB-CG	7.79	133.21	115.30
1	S2	959	U	C2-N1-C1'	7.78	127.04	117.70
86	A	1899	ALA	C-N-CA	7.76	141.11	121.70
40	LA	2836	C	N1-C2-O2	7.76	123.56	118.90
40	LA	3214	U	C2-N1-C1'	7.76	127.01	117.70
40	LA	2495	C	C2-N1-C1'	7.75	127.33	118.80
1	S2	1258	U	N1-C2-O2	7.74	128.22	122.80
86	A	2410	ALA	C-N-CA	7.74	141.06	121.70
40	LA	1716	U	P-O3'-C3'	7.74	128.99	119.70
36	Sm	49	G	C4-N9-C1'	7.73	136.56	126.50
86	A	2299	ALA	C-N-CA	7.73	141.03	121.70
40	LA	2257	C	N3-C2-O2	-7.71	116.50	121.90
1	S2	1145	U	C2-N1-C1'	7.71	126.95	117.70
40	LA	2434	U	C2-N1-C1'	7.70	126.94	117.70
1	S2	1633	A	P-O3'-C3'	7.70	128.94	119.70
40	LA	922	U	N1-C2-O2	7.69	128.18	122.80
1	S2	1256	A	P-O3'-C3'	7.69	128.92	119.70
40	LA	1604	G	N3-C4-C5	-7.68	124.76	128.60
1	S2	555	A	N7-C8-N9	7.68	117.64	113.80
40	LA	1614	C	C6-N1-C2	-7.68	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1202	A	C2-N3-C4	7.67	114.44	110.60
37	Sn	72	U	N3-C2-O2	-7.66	116.84	122.20
1	S2	583	C	C2-N1-C1'	7.66	127.22	118.80
1	S2	959	U	N1-C2-O2	7.65	128.15	122.80
40	LA	2531	C	C5-C6-N1	7.64	124.82	121.00
40	LA	2102	U	C5-C6-N1	7.64	126.52	122.70
40	LA	3217	C	C6-N1-C2	-7.64	117.24	120.30
1	S2	1258	U	C2-N1-C1'	7.63	126.86	117.70
6	SR	140	ARG	NE-CZ-NH2	-7.63	116.49	120.30
40	LA	3269	U	C2-N1-C1'	7.62	126.84	117.70
1	S2	453	U	N3-C2-O2	-7.62	116.87	122.20
1	S2	1389	C	C6-N1-C2	-7.61	117.25	120.30
40	LA	2132	C	C6-N1-C2	-7.60	117.26	120.30
37	Sn	63	G	OP1-P-O3'	7.58	121.88	105.20
40	LA	3181	C	N3-C2-O2	-7.58	116.60	121.90
1	S2	555	A	C8-N9-C4	-7.56	102.78	105.80
42	LC	125	U	C6-N1-C1'	-7.56	110.61	121.20
1	S2	225	A	C8-N9-C4	-7.56	102.78	105.80
1	S2	1527	C	N3-C2-O2	-7.56	116.61	121.90
1	S2	440	U	N1-C2-N3	7.55	119.43	114.90
1	S2	645	C	C6-N1-C2	-7.55	117.28	120.30
1	S2	276	C	N1-C2-O2	7.54	123.42	118.90
1	S2	1585	U	C5-C6-N1	7.53	126.47	122.70
40	LA	3131	U	C2-N1-C1'	7.53	126.74	117.70
40	LA	2492	C	C6-N1-C2	-7.52	117.29	120.30
40	LA	8	C	C6-N1-C2	-7.52	117.29	120.30
40	LA	2537	U	P-O3'-C3'	7.50	128.70	119.70
1	S2	656	G	N3-C4-C5	-7.50	124.85	128.60
1	S2	1374	C	C6-N1-C2	-7.50	117.30	120.30
1	S2	656	G	N3-C4-N9	7.49	130.50	126.00
40	LA	2389	C	C5-C6-N1	7.49	124.75	121.00
40	LA	1556	C	N1-C2-O2	7.49	123.39	118.90
40	LA	2873	U	N3-C2-O2	-7.49	116.96	122.20
36	Sm	56	C	N1-C2-O2	7.48	123.39	118.90
40	LA	3317	U	C2-N1-C1'	7.47	126.66	117.70
40	LA	2772	C	N1-C2-O2	7.46	123.38	118.90
40	LA	2531	C	C2-N1-C1'	7.45	127.00	118.80
40	LA	969	C	N3-C2-O2	-7.45	116.69	121.90
40	LA	1604	G	N3-C4-N9	7.41	130.45	126.00
40	LA	3218	A	OP2-P-O3'	7.40	121.49	105.20
40	LA	1155	C	C2-N1-C1'	7.40	126.94	118.80
36	Sm	49	G	N3-C4-C5	-7.40	124.90	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	2551	U	N3-C2-O2	-7.39	117.03	122.20
40	LA	2836	C	N3-C2-O2	-7.39	116.73	121.90
40	LA	492	C	C6-N1-C2	-7.37	117.35	120.30
1	S2	224	C	P-O3'-C3'	7.36	128.53	119.70
40	LA	3164	C	N3-C2-O2	-7.36	116.75	121.90
1	S2	1585	U	N1-C2-O2	7.35	127.95	122.80
40	LA	3306	U	N3-C2-O2	-7.35	117.06	122.20
1	S2	215	A	P-O3'-C3'	7.35	128.52	119.70
40	LA	118	U	N3-C2-O2	-7.34	117.06	122.20
84	Ls	102	LEU	CA-CB-CG	7.34	132.17	115.30
1	S2	440	U	N3-C2-O2	-7.33	117.07	122.20
40	LA	439	C	N1-C2-O2	7.32	123.29	118.90
40	LA	1227	C	N3-C2-O2	-7.32	116.78	121.90
1	S2	262	U	N1-C2-O2	7.31	127.92	122.80
40	LA	1604	G	C4-N9-C1'	7.31	136.00	126.50
40	LA	982	C	C2-N1-C1'	7.31	126.84	118.80
1	S2	361	C	C6-N1-C2	-7.30	117.38	120.30
1	S2	186	C	N1-C2-O2	7.29	123.27	118.90
40	LA	2551	U	N1-C2-O2	7.29	127.90	122.80
40	LA	1437	C	C2-N1-C1'	7.28	126.81	118.80
40	LA	2652	U	N3-C2-O2	-7.28	117.11	122.20
1	S2	1182	U	C2-N1-C1'	7.27	126.43	117.70
40	LA	444	U	N1-C2-O2	7.27	127.89	122.80
58	LS	41	ASP	CB-CG-OD1	7.26	124.84	118.30
1	S2	1458	G	C8-N9-C1'	-7.25	117.57	127.00
1	S2	237	C	N1-C2-O2	7.25	123.25	118.90
1	S2	874	C	C5-C6-N1	7.24	124.62	121.00
40	LA	2094	C	N3-C2-O2	-7.24	116.83	121.90
1	S2	639	U	P-O3'-C3'	7.24	128.38	119.70
40	LA	1279	C	C6-N1-C2	-7.23	117.41	120.30
40	LA	3277	U	C2-N1-C1'	7.21	126.36	117.70
40	LA	1349	G	C4-N9-C1'	7.20	135.85	126.50
40	LA	1279	C	C5-C6-N1	7.19	124.59	121.00
1	S2	617	U	C5-C6-N1	7.19	126.29	122.70
36	Sm	7	U	C2-N1-C1'	7.19	126.32	117.70
40	LA	1355	A	OP2-P-O3'	7.18	121.00	105.20
40	LA	1872	C	N1-C2-O2	7.18	123.21	118.90
1	S2	656	G	C8-N9-C1'	-7.17	117.67	127.00
1	S2	160	C	C6-N1-C2	-7.17	117.43	120.30
40	LA	1269	U	N1-C2-O2	7.16	127.81	122.80
40	LA	2514	U	P-O3'-C3'	7.16	128.29	119.70
1	S2	500	C	N1-C2-O2	7.15	123.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1458	G	N3-C4-C5	-7.14	125.03	128.60
40	LA	1815	U	P-O3'-C3'	7.12	128.25	119.70
1	S2	965	U	N3-C2-O2	-7.12	117.22	122.20
36	Sm	49	G	N3-C4-N9	7.12	130.27	126.00
1	S2	517	U	N1-C2-O2	7.11	127.77	122.80
11	SU	158	ASP	CB-CG-OD1	7.11	124.70	118.30
40	LA	2894	C	C6-N1-C2	-7.11	117.46	120.30
1	S2	185	U	C5-C6-N1	7.10	126.25	122.70
1	S2	1258	U	N3-C2-O2	-7.09	117.24	122.20
40	LA	406	G	O4'-C1'-N9	7.08	113.86	108.20
40	LA	982	C	N1-C2-O2	7.07	123.14	118.90
40	LA	1582	C	OP1-P-O3'	7.07	120.76	105.20
37	Sn	72	U	N1-C2-O2	7.06	127.74	122.80
40	LA	1562	C	P-O3'-C3'	7.05	128.16	119.70
1	S2	276	C	C6-N1-C2	-7.04	117.48	120.30
40	LA	3193	C	N1-C2-O2	7.03	123.12	118.90
1	S2	262	U	N3-C2-O2	-7.02	117.28	122.20
86	A	2232	ALA	C-N-CA	7.02	139.26	121.70
25	Sb	93	LEU	CA-CB-CG	7.02	131.45	115.30
86	A	2343	ALA	C-N-CA	7.02	139.25	121.70
86	A	1353	GLN	C-N-CA	7.02	139.25	121.70
86	A	2032	ALA	C-N-CA	7.02	139.24	121.70
1	S2	77	U	P-O3'-C3'	7.01	128.12	119.70
40	LA	2507	C	C5-C6-N1	7.01	124.51	121.00
40	LA	1280	C	N1-C2-O2	7.01	123.11	118.90
86	A	1832	ALA	C-N-CA	7.01	139.22	121.70
1	S2	1148	C	C6-N1-C2	-7.00	117.50	120.30
42	LC	64	U	N3-C2-O2	-7.00	117.30	122.20
41	LB	39	C	N3-C2-O2	-6.98	117.01	121.90
40	LA	1227	C	C6-N1-C2	-6.98	117.51	120.30
40	LA	763	G	P-O3'-C3'	6.98	128.07	119.70
40	LA	3269	U	N1-C2-O2	6.97	127.68	122.80
40	LA	1269	U	N3-C2-O2	-6.96	117.33	122.20
40	LA	1716	U	OP1-P-O3'	6.96	120.52	105.20
1	S2	1205	C	N1-C2-O2	6.95	123.07	118.90
1	S2	959	U	N3-C2-O2	-6.93	117.35	122.20
40	LA	3058	U	N1-C2-O2	6.93	127.65	122.80
40	LA	2407	C	C5-C6-N1	6.92	124.46	121.00
1	S2	530	C	N1-C2-O2	6.92	123.05	118.90
1	S2	1497	U	N1-C2-O2	6.92	127.64	122.80
37	Sn	34	C	C5-C6-N1	6.91	124.46	121.00
40	LA	142	C	C6-N1-C2	-6.91	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	Sn	46	G	C8-N9-C4	-6.90	103.64	106.40
40	LA	492	C	C5-C6-N1	6.88	124.44	121.00
1	S2	433	C	C5-C6-N1	6.88	124.44	121.00
40	LA	492	C	N1-C2-O2	6.88	123.03	118.90
41	LB	34	C	C6-N1-C2	-6.87	117.55	120.30
40	LA	2507	C	C6-N1-C2	-6.86	117.56	120.30
40	LA	3196	U	C2-N1-C1'	6.85	125.92	117.70
28	SK	77	ARG	NE-CZ-NH2	6.85	123.72	120.30
40	LA	3278	C	N3-C2-O2	-6.85	117.11	121.90
41	LB	52	G	P-O3'-C3'	6.85	127.92	119.70
6	SR	140	ARG	NE-CZ-NH1	6.84	123.72	120.30
27	Sd	74	LEU	CA-CB-CG	6.84	131.03	115.30
1	S2	758	U	N1-C2-O2	6.84	127.59	122.80
40	LA	922	U	N3-C2-O2	-6.84	117.41	122.20
1	S2	530	C	C6-N1-C2	-6.83	117.57	120.30
1	S2	934	C	C6-N1-C2	-6.83	117.57	120.30
1	S2	1585	U	N3-C4-O4	6.81	124.17	119.40
1	S2	1273	G	P-O3'-C3'	6.80	127.86	119.70
40	LA	2163	C	C6-N1-C2	-6.80	117.58	120.30
1	S2	322	G	P-O3'-C3'	6.80	127.86	119.70
1	S2	1220	C	C5-C6-N1	6.80	124.40	121.00
1	S2	1389	C	C5-C6-N1	6.79	124.39	121.00
86	A	2039	ALA	C-N-CA	6.79	138.67	121.70
40	LA	1283	C	C6-N1-C2	-6.78	117.59	120.30
1	S2	453	U	C6-N1-C2	-6.78	116.93	121.00
40	LA	2594	C	N1-C2-O2	6.78	122.97	118.90
86	A	2350	ALA	C-N-CA	6.78	138.64	121.70
1	S2	1382	A	P-O3'-C3'	6.78	127.83	119.70
86	A	1839	ALA	C-N-CA	6.78	138.64	121.70
86	A	2239	ALA	C-N-CA	6.78	138.64	121.70
1	S2	1182	U	N3-C2-O2	-6.76	117.47	122.20
40	LA	2112	U	P-O3'-C3'	6.76	127.82	119.70
1	S2	1220	C	C6-N1-C2	-6.76	117.60	120.30
40	LA	3078	U	OP2-P-O3'	6.75	120.04	105.20
16	SD	39	ASP	CB-CG-OD1	6.74	124.37	118.30
36	Sm	40	C	C6-N1-C2	-6.74	117.60	120.30
36	Sm	60	U	C5-C6-N1	6.74	126.07	122.70
40	LA	1496	C	C6-N1-C2	-6.74	117.60	120.30
40	LA	1597	C	C6-N1-C2	-6.74	117.60	120.30
40	LA	3058	U	C2-N1-C1'	6.74	125.79	117.70
40	LA	1574	C	N3-C2-O2	-6.73	117.19	121.90
40	LA	1907	C	N3-C2-O2	-6.73	117.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1528	U	N3-C2-O2	-6.73	117.49	122.20
40	LA	1608	C	C2-N1-C1'	6.73	126.20	118.80
40	LA	354	U	N1-C2-O2	6.73	127.51	122.80
40	LA	2407	C	C6-N1-C2	-6.73	117.61	120.30
40	LA	1437	C	C6-N1-C2	-6.72	117.61	120.30
40	LA	1706	C	C6-N1-C2	-6.72	117.61	120.30
1	S2	735	C	N1-C2-O2	6.71	122.93	118.90
40	LA	2666	C	C6-N1-C2	-6.70	117.62	120.30
1	S2	959	U	C5-C6-N1	6.70	126.05	122.70
40	LA	1556	C	C6-N1-C2	-6.70	117.62	120.30
40	LA	3217	C	C5-C6-N1	6.70	124.35	121.00
1	S2	139	C	P-O3'-C3'	6.68	127.72	119.70
40	LA	3196	U	N1-C2-O2	6.68	127.47	122.80
1	S2	711	U	P-O3'-C3'	6.66	127.70	119.70
1	S2	1633	A	OP2-P-O3'	6.66	119.85	105.20
40	LA	3097	C	C6-N1-C2	-6.65	117.64	120.30
42	LC	100	U	C2-N1-C1'	6.65	125.68	117.70
40	LA	1307	G	P-O3'-C3'	6.64	127.67	119.70
42	LC	125	U	C5-C6-N1	6.62	126.01	122.70
40	LA	2405	C	C2-N1-C1'	6.62	126.08	118.80
40	LA	3218	A	P-O3'-C3'	6.61	127.64	119.70
1	S2	1463	C	C6-N1-C2	-6.61	117.66	120.30
40	LA	2846	U	C2-N1-C1'	6.60	125.62	117.70
1	S2	14	C	C6-N1-C2	-6.60	117.66	120.30
1	S2	217	A	O5'-P-OP1	-6.60	99.76	105.70
40	LA	1283	C	C2-N1-C1'	6.59	126.06	118.80
1	S2	494	U	C2-N1-C1'	6.59	125.60	117.70
1	S2	583	C	C6-N1-C2	-6.58	117.67	120.30
40	LA	637	C	P-O3'-C3'	6.58	127.60	119.70
1	S2	120	U	N1-C2-O2	6.58	127.41	122.80
1	S2	1620	C	N1-C2-O2	6.58	122.85	118.90
40	LA	515	C	C6-N1-C2	-6.58	117.67	120.30
1	S2	640	U	P-O3'-C3'	6.58	127.59	119.70
1	S2	1274	C	P-O3'-C3'	6.58	127.59	119.70
1	S2	1389	C	N3-C2-O2	-6.58	117.30	121.90
40	LA	2552	C	N1-C2-O2	6.58	122.84	118.90
40	LA	3278	C	N1-C2-O2	6.58	122.84	118.90
1	S2	237	C	N3-C2-O2	-6.57	117.30	121.90
1	S2	608	U	C2-N1-C1'	6.57	125.58	117.70
1	S2	758	U	N3-C2-O2	-6.57	117.60	122.20
1	S2	489	C	C6-N1-C2	-6.57	117.67	120.30
40	LA	3306	U	N1-C2-O2	6.56	127.39	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	2492	C	C5-C6-N1	6.56	124.28	121.00
41	LB	105	C	N1-C2-O2	6.56	122.83	118.90
40	LA	3269	U	N3-C2-O2	-6.55	117.61	122.20
40	LA	2873	U	N1-C2-O2	6.55	127.39	122.80
1	S2	1560	U	N1-C2-O2	6.55	127.38	122.80
1	S2	1273	G	OP2-P-O3'	6.55	119.60	105.20
1	S2	1257	U	C2-N1-C1'	6.54	125.55	117.70
40	LA	2550	U	N3-C2-O2	-6.54	117.62	122.20
40	LA	2558	U	N3-C2-O2	-6.54	117.62	122.20
1	S2	1389	C	C6-N1-C1'	-6.54	112.96	120.80
1	S2	1657	U	N1-C2-O2	6.53	127.37	122.80
1	S2	1010	C	C6-N1-C2	-6.52	117.69	120.30
1	S2	1182	U	N1-C2-O2	6.52	127.36	122.80
1	S2	555	A	P-O3'-C3'	6.52	127.52	119.70
40	LA	3034	C	C6-N1-C2	-6.51	117.69	120.30
40	LA	1263	A	C2-N3-C4	6.51	113.86	110.60
1	S2	578	U	O5'-P-OP2	-6.50	99.85	105.70
1	S2	453	U	C5-C6-N1	6.50	125.95	122.70
28	SK	77	ARG	NE-CZ-NH1	-6.50	117.05	120.30
40	LA	78	U	N3-C2-O2	-6.50	117.65	122.20
41	LB	26	C	C6-N1-C2	-6.50	117.70	120.30
1	S2	1584	G	P-O3'-C3'	6.49	127.49	119.70
40	LA	2585	G	N3-C4-C5	-6.49	125.36	128.60
18	SZ	84	ARG	NE-CZ-NH2	-6.48	117.06	120.30
40	LA	667	C	C6-N1-C2	-6.48	117.71	120.30
1	S2	1075	C	C6-N1-C2	-6.48	117.71	120.30
36	Sm	60	U	C6-N1-C2	-6.47	117.12	121.00
1	S2	121	U	N3-C2-O2	-6.46	117.67	122.20
40	LA	439	C	N3-C2-O2	-6.46	117.38	121.90
40	LA	758	C	C6-N1-C2	-6.46	117.72	120.30
40	LA	2378	C	C2-N1-C1'	6.46	125.91	118.80
1	S2	141	U	P-O3'-C3'	6.46	127.45	119.70
36	Sm	57	G	P-O3'-C3'	6.46	127.45	119.70
1	S2	1216	C	N1-C2-O2	6.46	122.77	118.90
40	LA	2983	C	C2-N1-C1'	6.45	125.89	118.80
40	LA	800	G	N3-C4-C5	-6.44	125.38	128.60
40	LA	3195	U	C2-N1-C1'	6.44	125.43	117.70
1	S2	934	C	C5-C6-N1	6.43	124.22	121.00
40	LA	977	C	C5-C6-N1	6.43	124.22	121.00
40	LA	224	C	O5'-P-OP1	-6.43	99.91	105.70
40	LA	2836	C	C6-N1-C2	-6.43	117.73	120.30
1	S2	172	C	C2-N1-C1'	6.42	125.87	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	183	U	C5-C6-N1	6.42	125.91	122.70
1	S2	35	U	N3-C2-O2	-6.42	117.70	122.20
1	S2	583	C	N1-C2-O2	6.42	122.75	118.90
1	S2	1463	C	N1-C2-O2	6.42	122.75	118.90
1	S2	1279	C	C6-N1-C2	-6.42	117.73	120.30
41	LB	39	C	C6-N1-C2	-6.42	117.73	120.30
40	LA	700	C	C6-N1-C2	-6.42	117.73	120.30
40	LA	1556	C	N3-C2-O2	-6.42	117.41	121.90
40	LA	118	U	N1-C2-O2	6.41	127.29	122.80
40	LA	2422	C	C6-N1-C2	-6.41	117.73	120.30
1	S2	387	A	P-O3'-C3'	6.41	127.39	119.70
1	S2	1458	G	N3-C4-N9	6.41	129.85	126.00
42	LC	110	C	N1-C2-O2	6.40	122.74	118.90
37	Sn	34	C	C6-N1-C2	-6.40	117.74	120.30
1	S2	1082	C	N1-C2-O2	6.40	122.74	118.90
40	LA	3164	C	N1-C2-O2	6.40	122.74	118.90
1	S2	1527	C	C6-N1-C2	-6.40	117.74	120.30
36	Sm	16	U	C5-C6-N1	6.39	125.89	122.70
1	S2	870	C	C6-N1-C2	-6.39	117.75	120.30
1	S2	518	A	P-O3'-C3'	6.38	127.36	119.70
40	LA	2867	C	C6-N1-C2	-6.38	117.75	120.30
1	S2	590	C	C6-N1-C2	-6.38	117.75	120.30
40	LA	1333	C	C5-C6-N1	6.38	124.19	121.00
1	S2	1147	A	N7-C8-N9	6.38	116.99	113.80
40	LA	2513	U	OP1-P-O3'	6.38	119.24	105.20
1	S2	700	C	C5-C6-N1	6.38	124.19	121.00
1	S2	1307	U	N3-C2-O2	-6.38	117.73	122.20
40	LA	1820	U	OP2-P-O3'	6.38	119.23	105.20
40	LA	911	C	C6-N1-C2	-6.38	117.75	120.30
40	LA	97	U	N3-C2-O2	-6.37	117.74	122.20
1	S2	861	U	N1-C2-O2	6.37	127.26	122.80
1	S2	989	U	N1-C2-O2	6.37	127.26	122.80
40	LA	2552	C	C2-N1-C1'	6.36	125.80	118.80
1	S2	166	C	N1-C2-O2	6.36	122.72	118.90
40	LA	1854	C	C6-N1-C2	-6.36	117.76	120.30
1	S2	1161	C	C5-C6-N1	6.35	124.18	121.00
40	LA	1032	C	C6-N1-C2	-6.35	117.76	120.30
40	LA	1579	C	N1-C2-O2	6.34	122.70	118.90
1	S2	1497	U	N3-C2-O2	-6.34	117.76	122.20
37	Sn	25	C	C6-N1-C2	-6.34	117.76	120.30
40	LA	1118	C	C6-N1-C2	-6.34	117.76	120.30
40	LA	2237	C	N3-C2-O2	-6.33	117.47	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1556	A	P-O3'-C3'	6.33	127.30	119.70
40	LA	3097	C	C5-C6-N1	6.33	124.17	121.00
40	LA	2638	C	N1-C2-O2	6.33	122.70	118.90
36	Sm	61	C	N3-C2-O2	-6.33	117.47	121.90
1	S2	433	C	C6-N1-C2	-6.33	117.77	120.30
36	Sm	16	U	C6-N1-C2	-6.33	117.20	121.00
40	LA	2094	C	N1-C2-O2	6.33	122.69	118.90
40	LA	3194	C	N1-C2-O2	6.32	122.69	118.90
1	S2	1489	U	C2-N1-C1'	6.32	125.28	117.70
1	S2	1632	C	N1-C2-O2	6.32	122.69	118.90
40	LA	1224	C	C6-N1-C2	-6.32	117.77	120.30
62	LW	50	LEU	CA-CB-CG	6.32	129.84	115.30
40	LA	849	C	P-O3'-C3'	6.32	127.28	119.70
40	LA	1155	C	C6-N1-C2	-6.31	117.78	120.30
40	LA	2889	C	C6-N1-C2	-6.31	117.78	120.30
40	LA	1275	C	N3-C2-O2	-6.30	117.49	121.90
1	S2	1674	C	C6-N1-C2	-6.30	117.78	120.30
40	LA	263	C	C6-N1-C2	-6.30	117.78	120.30
40	LA	3153	U	O4'-C1'-N1	6.30	113.24	108.20
1	S2	445	A	C2-N3-C4	6.29	113.75	110.60
1	S2	1573	A	P-O3'-C3'	6.29	127.24	119.70
1	S2	139	C	OP2-P-O3'	6.28	119.02	105.20
40	LA	2496	C	C6-N1-C2	-6.28	117.79	120.30
40	LA	3278	C	C2-N1-C1'	6.27	125.70	118.80
1	S2	440	U	C2-N3-C4	-6.26	123.24	127.00
1	S2	864	U	C2-N1-C1'	6.26	125.22	117.70
40	LA	2194	G	N3-C4-N9	6.26	129.76	126.00
36	Sm	56	C	N3-C2-O2	-6.26	117.52	121.90
40	LA	2237	C	N1-C2-O2	6.26	122.66	118.90
40	LA	1878	G	C4-N9-C1'	6.25	134.63	126.50
1	S2	1201	G	OP1-P-O3'	6.25	118.94	105.20
40	LA	1278	A	O4'-C1'-N9	6.25	113.20	108.20
40	LA	1448	U	C2-N1-C1'	6.24	125.19	117.70
40	LA	2257	C	C6-N1-C2	-6.24	117.81	120.30
1	S2	120	U	N3-C2-O2	-6.23	117.84	122.20
42	LC	100	U	N1-C2-O2	6.22	127.16	122.80
1	S2	530	C	N3-C2-O2	-6.21	117.55	121.90
40	LA	753	C	C6-N1-C2	-6.21	117.81	120.30
1	S2	120	U	C2-N1-C1'	6.20	125.14	117.70
42	LC	21	C	C2-N1-C1'	6.20	125.62	118.80
1	S2	755	A	P-O3'-C3'	6.20	127.14	119.70
1	S2	861	U	C6-N1-C1'	-6.20	112.52	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	2622	C	N1-C2-O2	6.20	122.62	118.90
1	S2	453	U	N1-C2-O2	6.20	127.14	122.80
40	LA	332	C	C6-N1-C2	-6.20	117.82	120.30
1	S2	1222	C	C6-N1-C2	-6.20	117.82	120.30
40	LA	2257	C	C6-N1-C1'	-6.20	113.37	120.80
1	S2	278	U	P-O3'-C3'	6.19	127.13	119.70
36	Sm	49	G	C8-N9-C1'	-6.19	118.95	127.00
40	LA	860	G	C2-N3-C4	6.19	115.00	111.90
40	LA	1222	G	O4'-C1'-N9	6.19	113.16	108.20
30	Sf	41	LEU	CA-CB-CG	6.19	129.53	115.30
1	S2	767	U	C2-N1-C1'	6.19	125.12	117.70
1	S2	138	A	C2-N3-C4	6.18	113.69	110.60
36	Sm	62	C	C6-N1-C1'	6.18	128.22	120.80
1	S2	530	C	C2-N1-C1'	6.18	125.60	118.80
1	S2	1274	C	OP2-P-O3'	6.18	118.79	105.20
40	LA	2098	C	C6-N1-C2	-6.17	117.83	120.30
40	LA	2388	U	N3-C2-O2	-6.17	117.88	122.20
1	S2	1657	U	N3-C2-O2	-6.17	117.88	122.20
40	LA	15	C	C6-N1-C2	-6.17	117.83	120.30
1	S2	965	U	C6-N1-C1'	-6.16	112.57	121.20
40	LA	2176	U	C5-C6-N1	6.16	125.78	122.70
1	S2	1251	U	P-O3'-C3'	6.16	127.09	119.70
1	S2	1585	U	N3-C2-O2	-6.16	117.89	122.20
40	LA	663	C	C6-N1-C2	-6.16	117.84	120.30
1	S2	1307	U	N1-C2-O2	6.15	127.11	122.80
42	LC	85	G	P-O3'-C3'	6.15	127.08	119.70
40	LA	2712	U	C2-N1-C1'	6.14	125.07	117.70
36	Sm	48	C	P-O3'-C3'	6.14	127.07	119.70
42	LC	64	U	N1-C2-O2	6.14	127.10	122.80
1	S2	400	A	OP2-P-O3'	6.14	118.71	105.20
40	LA	379	C	C6-N1-C2	-6.14	117.84	120.30
40	LA	118	U	C2-N1-C1'	6.14	125.06	117.70
1	S2	1585	U	C5-C4-O4	-6.13	122.22	125.90
40	LA	1228	C	C6-N1-C2	-6.13	117.85	120.30
40	LA	1604	G	C8-N9-C1'	-6.13	119.03	127.00
1	S2	186	C	C6-N1-C2	-6.13	117.85	120.30
1	S2	1248	C	C6-N1-C2	-6.13	117.85	120.30
40	LA	1496	C	C5-C6-N1	6.13	124.06	121.00
1	S2	283	U	N1-C2-O2	6.12	127.08	122.80
40	LA	2806	U	O5'-P-OP1	-6.12	100.19	105.70
1	S2	54	C	C6-N1-C2	-6.11	117.85	120.30
42	LC	115	C	C6-N1-C2	-6.11	117.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	3089	C	C6-N1-C2	-6.11	117.86	120.30
40	LA	1275	C	N1-C2-O2	6.11	122.56	118.90
40	LA	1604	G	C2-N3-C4	6.11	114.95	111.90
40	LA	1508	C	N1-C2-O2	6.10	122.56	118.90
1	S2	803	A	P-O3'-C3'	6.10	127.02	119.70
84	Ls	39	CYS	CA-CB-SG	6.10	124.99	114.00
40	LA	2551	U	C2-N1-C1'	6.10	125.02	117.70
40	LA	663	C	C5-C6-N1	6.10	124.05	121.00
40	LA	3195	U	N1-C2-O2	6.10	127.07	122.80
1	S2	1205	C	C2-N1-C1'	6.09	125.50	118.80
1	S2	1214	U	N1-C2-O2	6.09	127.06	122.80
40	LA	1608	C	N1-C2-O2	6.09	122.56	118.90
40	LA	3228	C	P-O3'-C3'	6.09	127.01	119.70
42	LC	100	U	N3-C2-O2	-6.09	117.94	122.20
1	S2	1491	U	C2-N1-C1'	6.09	125.00	117.70
40	LA	2378	C	N1-C2-O2	6.09	122.55	118.90
40	LA	2899	C	C2-N1-C1'	6.08	125.49	118.80
1	S2	1463	C	C5-C6-N1	6.08	124.04	121.00
1	S2	1560	U	O4'-C1'-N1	6.08	113.06	108.20
40	LA	2726	C	C2-N1-C1'	6.07	125.48	118.80
36	Sm	61	C	N1-C2-O2	6.07	122.54	118.90
40	LA	2773	C	N1-C2-O2	6.07	122.54	118.90
40	LA	2585	G	N3-C4-N9	6.06	129.63	126.00
1	S2	928	U	P-O3'-C3'	6.05	126.96	119.70
86	A	1615	ALA	O-C-N	-6.05	113.01	122.70
40	LA	2941	A	O5'-P-OP1	-6.05	100.25	105.70
40	LA	1278	A	C8-N9-C4	-6.05	103.38	105.80
1	S2	1363	U	N1-C2-O2	6.05	127.03	122.80
1	S2	767	U	N1-C2-O2	6.05	127.03	122.80
40	LA	1878	G	C8-N9-C1'	-6.04	119.14	127.00
1	S2	160	C	C2-N1-C1'	6.04	125.44	118.80
1	S2	989	U	N3-C2-O2	-6.03	117.98	122.20
1	S2	989	U	C2-N1-C1'	6.03	124.94	117.70
40	LA	3196	U	N3-C2-O2	-6.03	117.98	122.20
40	LA	3269	U	OP2-P-O3'	6.03	118.46	105.20
40	LA	1583	A	O5'-P-OP1	-6.02	100.28	105.70
40	LA	87	U	C2-N1-C1'	6.02	124.92	117.70
40	LA	969	C	C6-N1-C2	-6.02	117.89	120.30
40	LA	1349	G	C2-N3-C4	6.02	114.91	111.90
40	LA	1943	C	C6-N1-C2	-6.02	117.89	120.30
40	LA	3078	U	P-O3'-C3'	6.02	126.92	119.70
40	LA	2664	C	C2-N1-C1'	6.01	125.42	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	SW	132	ARG	CA-CB-CG	6.01	126.63	113.40
40	LA	1581	C	C6-N1-C2	-6.01	117.89	120.30
1	S2	186	C	C5-C6-N1	6.01	124.00	121.00
40	LA	860	G	N3-C2-N2	-6.00	115.70	119.90
1	S2	705	U	P-O3'-C3'	6.00	126.90	119.70
36	Sm	72	C	C2-N1-C1'	6.00	125.40	118.80
40	LA	1597	C	C5-C6-N1	6.00	124.00	121.00
36	Sm	46	G	OP1-P-OP2	-6.00	110.60	119.60
1	S2	1205	C	N3-C2-O2	-6.00	117.70	121.90
21	SH	112	ASP	CB-CG-OD1	6.00	123.70	118.30
40	LA	1437	C	N1-C2-O2	5.99	122.50	118.90
40	LA	1097	G	P-O3'-C3'	5.99	126.89	119.70
40	LA	803	C	C6-N1-C2	-5.99	117.91	120.30
41	LB	68	C	C6-N1-C2	-5.98	117.91	120.30
1	S2	583	C	C5-C6-N1	5.98	123.99	121.00
40	LA	3181	C	C6-N1-C2	-5.98	117.91	120.30
1	S2	1636	C	P-O3'-C3'	5.97	126.87	119.70
1	S2	1197	C	C6-N1-C2	-5.97	117.91	120.30
1	S2	1226	A	P-O3'-C3'	5.97	126.86	119.70
1	S2	1657	U	C2-N1-C1'	5.97	124.86	117.70
1	S2	88	U	N3-C2-O2	-5.95	118.03	122.20
33	SN	103	LEU	CA-CB-CG	5.95	128.99	115.30
1	S2	161	U	N3-C2-O2	-5.95	118.03	122.20
1	S2	1170	G	C4-N9-C1'	5.95	134.24	126.50
40	LA	1333	C	C6-N1-C2	-5.95	117.92	120.30
70	Le	104	LEU	CA-CB-CG	5.95	128.98	115.30
1	S2	1012	U	N3-C4-O4	5.94	123.56	119.40
40	LA	922	U	C6-N1-C1'	-5.94	112.88	121.20
40	LA	2652	U	N1-C2-O2	5.94	126.96	122.80
1	S2	700	C	C6-N1-C2	-5.94	117.92	120.30
40	LA	3214	U	N3-C2-O2	-5.94	118.04	122.20
40	LA	87	U	N1-C2-O2	5.94	126.95	122.80
40	LA	524	U	N1-C2-O2	5.94	126.95	122.80
1	S2	361	C	C5-C6-N1	5.93	123.97	121.00
37	Sn	76	A	O4'-C1'-N9	5.93	112.95	108.20
40	LA	2132	C	N3-C2-O2	-5.93	117.75	121.90
1	S2	736	C	C6-N1-C2	-5.93	117.93	120.30
1	S2	1063	U	N1-C2-O2	5.93	126.95	122.80
40	LA	3111	U	C5-C6-N1	5.93	125.66	122.70
1	S2	819	G	P-O3'-C3'	5.93	126.81	119.70
1	S2	1596	C	C2-N1-C1'	5.92	125.32	118.80
40	LA	2846	U	N3-C2-O2	-5.92	118.05	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	2849	C	C6-N1-C2	-5.92	117.93	120.30
40	LA	1309	U	N3-C2-O2	-5.92	118.06	122.20
40	LA	1064	A	P-O3'-C3'	5.92	126.80	119.70
1	S2	1216	C	N3-C2-O2	-5.91	117.76	121.90
1	S2	908	U	N3-C2-O2	-5.91	118.07	122.20
1	S2	224	C	N3-C2-O2	-5.90	117.77	121.90
40	LA	2788	C	C6-N1-C2	-5.90	117.94	120.30
40	LA	1227	C	C2-N1-C1'	5.90	125.29	118.80
1	S2	283	U	N3-C2-O2	-5.90	118.07	122.20
52	LM	117	ASP	CB-CG-OD1	5.90	123.61	118.30
40	LA	2422	C	C5-C6-N1	5.89	123.95	121.00
40	LA	3350	C	P-O3'-C3'	5.89	126.77	119.70
40	LA	543	C	N3-C2-O2	-5.89	117.78	121.90
36	Sm	65	C	C6-N1-C2	-5.88	117.95	120.30
1	S2	1451	C	C6-N1-C2	-5.88	117.95	120.30
1	S2	1510	U	C5-C6-N1	5.87	125.64	122.70
36	Sm	67	C	C6-N1-C2	-5.87	117.95	120.30
40	LA	8	C	C5-C6-N1	5.87	123.94	121.00
1	S2	1596	C	O4'-C1'-N1	5.87	112.90	108.20
40	LA	444	U	C6-N1-C2	-5.87	117.48	121.00
1	S2	411	C	C6-N1-C2	-5.86	117.95	120.30
37	Sn	71	C	C6-N1-C2	-5.86	117.95	120.30
40	LA	3214	U	N1-C2-O2	5.85	126.90	122.80
40	LA	700	C	C5-C6-N1	5.85	123.93	121.00
40	LA	2405	C	N3-C2-O2	-5.85	117.80	121.90
40	LA	3153	U	C2-N1-C1'	5.85	124.72	117.70
40	LA	2712	U	N1-C2-O2	5.85	126.89	122.80
40	LA	3181	C	C6-N1-C1'	-5.85	113.78	120.80
1	S2	1082	C	C6-N1-C1'	-5.85	113.78	120.80
40	LA	1349	G	C8-N9-C1'	-5.84	119.40	127.00
40	LA	915	A	N7-C8-N9	5.84	116.72	113.80
40	LA	2406	C	C6-N1-C2	-5.84	117.97	120.30
40	LA	2550	U	C2-N1-C1'	5.84	124.71	117.70
40	LA	1660	C	C6-N1-C2	-5.84	117.97	120.30
1	S2	305	C	C6-N1-C2	-5.83	117.97	120.30
1	S2	1246	C	N1-C2-O2	5.83	122.40	118.90
1	S2	908	U	N1-C2-O2	5.83	126.88	122.80
36	Sm	53	G	N1-C6-O6	-5.82	116.41	119.90
40	LA	2514	U	OP1-P-O3'	5.82	118.01	105.20
40	LA	2137	U	C2-N1-C1'	5.82	124.68	117.70
1	S2	840	U	N3-C2-O2	-5.82	118.13	122.20
40	LA	1872	C	N3-C2-O2	-5.82	117.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	3269	U	P-O3'-C3'	5.82	126.68	119.70
44	LE	291	GLU	CA-CB-CG	5.82	126.19	113.40
1	S2	322	G	OP2-P-O3'	5.81	117.98	105.20
40	LA	2445	A	P-O3'-C3'	5.81	126.67	119.70
40	LA	2541	U	N1-C2-O2	5.81	126.86	122.80
40	LA	2889	C	C5-C6-N1	5.81	123.90	121.00
1	S2	507	U	C6-N1-C2	-5.80	117.52	121.00
40	LA	3350	C	C6-N1-C2	-5.80	117.98	120.30
40	LA	1355	A	P-O3'-C3'	5.80	126.66	119.70
1	S2	1245	G	P-O3'-C3'	5.80	126.66	119.70
37	Sn	50	U	O5'-P-OP2	-5.79	100.49	105.70
68	Lc	46	ASP	CB-CG-OD1	5.79	123.52	118.30
40	LA	2764	C	C6-N1-C2	-5.79	117.98	120.30
46	LG	137	ASP	CB-CG-OD1	5.79	123.51	118.30
1	S2	262	U	C2-N1-C1'	5.79	124.65	117.70
18	SZ	84	ARG	NE-CZ-NH1	5.79	123.19	120.30
40	LA	1155	C	N1-C2-O2	5.78	122.37	118.90
40	LA	1574	C	N1-C2-O2	5.78	122.37	118.90
1	S2	849	C	C6-N1-C2	-5.78	117.99	120.30
1	S2	803	A	OP2-P-O3'	5.78	117.92	105.20
1	S2	629	U	N3-C2-O2	-5.78	118.15	122.20
40	LA	2102	U	O4'-C1'-N1	5.78	112.82	108.20
1	S2	313	U	P-O3'-C3'	5.78	126.63	119.70
40	LA	1470	U	N3-C2-O2	-5.78	118.16	122.20
1	S2	1451	C	C5-C6-N1	5.77	123.89	121.00
40	LA	855	U	C2-N1-C1'	5.77	124.63	117.70
84	Ls	111	ASP	C-N-CA	5.77	136.12	121.70
40	LA	586	C	C6-N1-C2	-5.76	117.99	120.30
40	LA	1508	C	C6-N1-C2	-5.76	117.99	120.30
40	LA	1280	C	C6-N1-C2	-5.76	118.00	120.30
40	LA	3120	C	O5'-P-OP2	-5.76	100.51	105.70
1	S2	1560	U	C6-N1-C2	-5.76	117.55	121.00
1	S2	1161	C	C6-N1-C2	-5.75	118.00	120.30
40	LA	3155	U	N1-C2-O2	5.75	126.82	122.80
1	S2	1583	A	O4'-C1'-N9	5.75	112.80	108.20
40	LA	356	C	C6-N1-C2	-5.75	118.00	120.30
17	SY	56	ASP	CB-CG-OD1	5.74	123.47	118.30
1	S2	1214	U	N3-C2-O2	-5.74	118.18	122.20
47	LH	77	ARG	N-CA-CB	5.74	120.93	110.60
1	S2	1082	C	O4'-C1'-N1	5.74	112.79	108.20
40	LA	2434	U	C6-N1-C2	-5.74	117.56	121.00
40	LA	3363	U	N3-C2-O2	-5.74	118.19	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	515	C	C5-C6-N1	5.73	123.87	121.00
34	SO	42	LEU	CA-CB-CG	5.73	128.48	115.30
1	S2	1314	U	OP2-P-O3'	5.73	117.80	105.20
40	LA	3076	C	C6-N1-C2	-5.73	118.01	120.30
1	S2	1641	C	C6-N1-C2	-5.73	118.01	120.30
1	S2	927	C	C6-N1-C2	-5.72	118.01	120.30
40	LA	1746	U	N3-C2-O2	-5.72	118.20	122.20
1	S2	861	U	N3-C2-O2	-5.71	118.20	122.20
41	LB	78	U	N1-C2-O2	5.71	126.80	122.80
40	LA	2594	C	N3-C2-O2	-5.71	117.90	121.90
40	LA	2336	U	N3-C2-O2	-5.71	118.20	122.20
1	S2	1602	C	C6-N1-C2	-5.71	118.02	120.30
21	SH	3	LEU	CA-CB-CG	5.71	128.43	115.30
41	LB	19	C	C6-N1-C2	-5.71	118.02	120.30
1	S2	482	U	N3-C2-O2	-5.70	118.21	122.20
40	LA	1516	C	C6-N1-C2	-5.70	118.02	120.30
36	Sm	63	U	C5-C6-N1	5.70	125.55	122.70
40	LA	1844	C	C6-N1-C2	-5.70	118.02	120.30
40	LA	3193	C	C6-N1-C2	-5.70	118.02	120.30
40	LA	444	U	C5-C6-N1	5.70	125.55	122.70
1	S2	1620	C	C2-N1-C1'	5.69	125.06	118.80
1	S2	267	U	N3-C2-O2	-5.69	118.22	122.20
40	LA	1208	U	N1-C2-O2	5.69	126.78	122.80
40	LA	1609	C	C6-N1-C2	-5.69	118.02	120.30
40	LA	13	A	OP2-P-O3'	5.69	117.71	105.20
40	LA	2277	C	C6-N1-C2	-5.69	118.03	120.30
68	Lc	81	LEU	CA-CB-CG	5.69	128.38	115.30
40	LA	1307	G	OP2-P-O3'	5.68	117.69	105.20
1	S2	121	U	C2-N1-C1'	5.67	124.51	117.70
1	S2	627	C	C2-N1-C1'	5.67	125.04	118.80
40	LA	2505	U	N3-C2-O2	-5.67	118.23	122.20
1	S2	911	U	N1-C2-O2	5.67	126.77	122.80
40	LA	800	G	N3-C4-N9	5.67	129.40	126.00
73	Lh	86	ARG	CA-CB-CG	5.67	125.87	113.40
1	S2	1528	U	N1-C2-O2	5.66	126.77	122.80
40	LA	3193	C	N3-C2-O2	-5.66	117.94	121.90
40	LA	1103	A	C2-N3-C4	5.66	113.43	110.60
1	S2	31	C	C6-N1-C2	-5.65	118.04	120.30
40	LA	2146	C	C6-N1-C2	-5.65	118.04	120.30
1	S2	494	U	N1-C2-O2	5.65	126.75	122.80
1	S2	1332	C	N1-C2-O2	5.65	122.29	118.90
40	LA	3235	C	C2-N1-C1'	5.65	125.01	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	3155	U	N3-C2-O2	-5.64	118.25	122.20
1	S2	1355	C	C6-N1-C2	-5.64	118.04	120.30
41	LB	39	C	C2-N1-C1'	5.64	125.00	118.80
40	LA	1224	C	C5-C6-N1	5.64	123.82	121.00
36	Sm	56	C	C6-N1-C2	-5.63	118.05	120.30
36	Sm	59	A	P-O3'-C3'	5.63	126.46	119.70
40	LA	2795	U	O5'-P-OP2	-5.63	100.63	105.70
1	S2	1528	U	O5'-P-OP2	-5.63	100.63	105.70
1	S2	645	C	C5-C6-N1	5.62	123.81	121.00
11	SU	38	LEU	CA-CB-CG	5.62	128.23	115.30
40	LA	2567	C	C6-N1-C2	-5.62	118.05	120.30
40	LA	249	U	N3-C2-O2	-5.62	118.27	122.20
1	S2	893	U	N3-C2-O2	-5.61	118.27	122.20
1	S2	1007	C	C6-N1-C2	-5.61	118.05	120.30
40	LA	2846	U	N1-C2-O2	5.61	126.73	122.80
40	LA	379	C	C5-C6-N1	5.61	123.81	121.00
37	Sn	32	C	N1-C2-O2	5.61	122.27	118.90
1	S2	283	U	C2-N1-C1'	5.61	124.43	117.70
1	S2	185	U	C6-N1-C2	-5.61	117.64	121.00
40	LA	3277	U	N3-C2-O2	-5.61	118.28	122.20
40	LA	1032	C	C5-C6-N1	5.60	123.80	121.00
1	S2	225	A	C6-C5-N7	-5.59	128.38	132.30
1	S2	1688	U	N1-C2-O2	5.59	126.72	122.80
40	LA	50	U	N1-C2-O2	5.59	126.71	122.80
40	LA	1508	C	N3-C2-O2	-5.59	117.99	121.90
21	SH	117	LYS	CD-CE-NZ	5.59	124.55	111.70
36	Sm	75	C	C6-N1-C2	-5.59	118.06	120.30
40	LA	354	U	N3-C2-O2	-5.59	118.29	122.20
40	LA	1433	A	O4'-C1'-N9	-5.59	103.73	108.20
1	S2	1711	C	C6-N1-C2	-5.59	118.07	120.30
40	LA	1076	C	C6-N1-C2	-5.59	118.06	120.30
40	LA	40	A	O4'-C1'-N9	5.58	112.67	108.20
40	LA	1722	U	N1-C2-O2	5.58	126.71	122.80
1	S2	1646	C	N1-C2-O2	5.58	122.25	118.90
1	S2	405	C	C6-N1-C2	-5.58	118.07	120.30
1	S2	1688	U	C2-N1-C1'	5.57	124.39	117.70
40	LA	398	A	O4'-C1'-N9	5.57	112.66	108.20
40	LA	2772	C	C6-N1-C1'	-5.57	114.12	120.80
1	S2	172	C	C6-N1-C2	-5.57	118.07	120.30
40	LA	543	C	N1-C2-O2	5.57	122.24	118.90
40	LA	2495	C	C6-N1-C1'	-5.57	114.12	120.80
1	S2	185	U	C2-N1-C1'	5.57	124.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1033	C	C6-N1-C2	-5.57	118.07	120.30
40	LA	225	C	C6-N1-C2	-5.56	118.08	120.30
86	A	1181	GLU	C-N-CA	5.56	145.35	122.00
40	LA	2349	U	C2-N1-C1'	5.56	124.37	117.70
40	LA	2585	G	C4-N9-C1'	5.56	133.73	126.50
40	LA	1496	C	N1-C2-O2	5.55	122.23	118.90
40	LA	228	U	C5-C6-N1	5.55	125.48	122.70
40	LA	1907	C	C2-N1-C1'	5.55	124.91	118.80
84	Ls	103	MET	CB-CG-SD	5.55	129.05	112.40
1	S2	1688	U	N3-C2-O2	-5.55	118.32	122.20
40	LA	36	C	C6-N1-C2	-5.54	118.08	120.30
40	LA	2359	C	C5-C6-N1	5.54	123.77	121.00
1	S2	609	U	OP2-P-O3'	5.54	117.39	105.20
1	S2	1252	C	C6-N1-C2	-5.54	118.08	120.30
40	LA	36	C	N3-C2-O2	-5.54	118.02	121.90
1	S2	555	A	C4-N9-C1'	5.54	136.27	126.30
40	LA	1581	C	N1-C2-O2	5.54	122.22	118.90
1	S2	1439	C	C6-N1-C2	-5.54	118.09	120.30
1	S2	1756	A	OP2-P-O3'	5.54	117.38	105.20
86	A	1162	ALA	C-N-CA	5.53	135.53	121.70
1	S2	1363	U	N3-C2-O2	-5.53	118.33	122.20
40	LA	2772	C	N3-C2-O2	-5.53	118.03	121.90
1	S2	883	C	C6-N1-C2	-5.53	118.09	120.30
40	LA	979	U	N3-C2-O2	-5.53	118.33	122.20
40	LA	1889	G	C4-N9-C1'	5.53	133.68	126.50
40	LA	1499	C	C6-N1-C2	-5.52	118.09	120.30
1	S2	189	C	C6-N1-C2	-5.52	118.09	120.30
37	Sn	25	C	N1-C2-O2	5.52	122.21	118.90
40	LA	2434	U	C5-C6-N1	5.52	125.46	122.70
40	LA	192	C	C6-N1-C2	-5.52	118.09	120.30
40	LA	855	U	N1-C2-O2	5.51	126.66	122.80
40	LA	1562	C	C3'-C2'-C1'	5.51	105.91	101.50
40	LA	2638	C	C6-N1-C2	-5.51	118.09	120.30
40	LA	3235	C	C6-N1-C2	-5.51	118.09	120.30
40	LA	3164	C	C6-N1-C2	-5.51	118.09	120.30
40	LA	3058	U	N3-C2-O2	-5.51	118.34	122.20
40	LA	2622	C	N3-C2-O2	-5.51	118.04	121.90
40	LA	2274	U	N1-C2-O2	5.51	126.66	122.80
40	LA	1684	U	C5-C6-N1	5.50	125.45	122.70
40	LA	2664	C	C5-C6-N1	5.50	123.75	121.00
40	LA	2894	C	C5-C6-N1	5.50	123.75	121.00
1	S2	735	C	N3-C2-O2	-5.49	118.06	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	LB	105	C	N3-C2-O2	-5.49	118.06	121.90
1	S2	1315	U	OP1-P-OP2	-5.49	111.37	119.60
1	S2	425	A	OP2-P-O3'	5.49	117.27	105.20
40	LA	1227	C	C5-C6-N1	5.49	123.74	121.00
1	S2	759	U	N3-C2-O2	-5.48	118.37	122.20
40	LA	969	C	C2-N1-C1'	5.48	124.83	118.80
40	LA	2567	C	C2-N1-C1'	5.48	124.82	118.80
40	LA	1901	A	C2-N3-C4	5.47	113.34	110.60
40	LA	2666	C	C5-C6-N1	5.47	123.74	121.00
1	S2	275	C	N1-C2-O2	5.47	122.18	118.90
1	S2	1248	C	C5-C6-N1	5.47	123.73	121.00
40	LA	3155	U	C2-N1-C1'	5.47	124.26	117.70
40	LA	1448	U	N1-C2-O2	5.47	126.63	122.80
35	SL	66	LEU	CA-CB-CG	5.46	127.87	115.30
40	LA	2842	U	N1-C2-O2	5.46	126.62	122.80
1	S2	1363	U	C2-N1-C1'	5.46	124.26	117.70
40	LA	439	C	OP1-P-O3'	5.46	117.22	105.20
1	S2	1706	C	C6-N1-C2	-5.46	118.12	120.30
1	S2	617	U	C2-N1-C1'	5.46	124.25	117.70
40	LA	1920	U	OP2-P-O3'	5.46	117.21	105.20
24	Sa	10	GLU	CA-CB-CG	5.46	125.41	113.40
40	LA	2495	C	N3-C2-O2	-5.46	118.08	121.90
40	LA	2955	U	C5-C6-N1	5.46	125.43	122.70
75	Lj	92	LEU	CA-CB-CG	5.46	127.85	115.30
40	LA	1279	C	N1-C2-O2	5.45	122.17	118.90
1	S2	1489	U	N1-C2-O2	5.45	126.61	122.80
1	S2	1205	C	C6-N1-C2	-5.45	118.12	120.30
40	LA	529	A	N7-C8-N9	5.44	116.52	113.80
1	S2	1461	C	C6-N1-C2	-5.44	118.12	120.30
12	SV	29	LEU	CA-CB-CG	5.43	127.79	115.30
40	LA	1037	C	C6-N1-C2	-5.43	118.13	120.30
1	S2	766	U	OP1-P-O3'	5.43	117.14	105.20
40	LA	2806	U	C5-C6-N1	5.43	125.42	122.70
40	LA	298	U	N1-C2-O2	5.43	126.60	122.80
40	LA	2496	C	N3-C2-O2	-5.43	118.10	121.90
33	SN	136	LYS	CA-CB-CG	5.42	125.33	113.40
40	LA	702	C	C6-N1-C2	-5.42	118.13	120.30
40	LA	915	A	C2-N3-C4	5.42	113.31	110.60
40	LA	1684	U	N3-C2-O2	-5.42	118.41	122.20
40	LA	2594	C	C2-N1-C1'	5.42	124.76	118.80
40	LA	190	U	OP2-P-O3'	5.42	117.12	105.20
40	LA	3195	U	N3-C2-O2	-5.42	118.41	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	LB	26	C	C5-C6-N1	5.42	123.71	121.00
1	S2	1201	G	P-O3'-C3'	5.41	126.20	119.70
40	LA	1146	C	C6-N1-C2	-5.41	118.14	120.30
40	LA	1706	C	N1-C2-O2	5.41	122.15	118.90
40	LA	596	C	C5-C6-N1	5.41	123.71	121.00
40	LA	2506	U	N3-C2-O2	-5.41	118.41	122.20
40	LA	1271	A	OP1-P-O3'	5.41	117.10	105.20
40	LA	2516	U	C5-C6-N1	5.41	125.40	122.70
1	S2	1032	G	O5'-P-OP2	-5.41	100.83	105.70
40	LA	1531	C	C6-N1-C2	-5.40	118.14	120.30
40	LA	3117	C	N1-C2-O2	5.40	122.14	118.90
40	LA	36	C	N1-C2-O2	5.40	122.14	118.90
1	S2	1514	U	N3-C2-O2	-5.39	118.43	122.20
11	SU	128	ASP	CB-CG-OD1	5.39	123.15	118.30
40	LA	1309	U	N1-C2-O2	5.39	126.57	122.80
40	LA	915	A	C8-N9-C4	-5.39	103.64	105.80
1	S2	1115	U	C5-C6-N1	5.38	125.39	122.70
37	Sn	49	C	C2-N1-C1'	5.38	124.72	118.80
1	S2	161	U	N1-C2-O2	5.38	126.57	122.80
1	S2	494	U	N3-C2-O2	-5.38	118.43	122.20
40	LA	2664	C	C6-N1-C2	-5.38	118.15	120.30
40	LA	3228	C	OP2-P-O3'	5.38	117.03	105.20
40	LA	3320	A	O5'-P-OP1	-5.38	100.86	105.70
42	LC	125	U	C6-N1-C2	-5.38	117.77	121.00
41	LB	116	C	C6-N1-C2	-5.38	118.15	120.30
40	LA	1278	A	N7-C8-N9	5.38	116.49	113.80
34	SO	33	LEU	CA-CB-CG	5.37	127.66	115.30
83	Lr	85	ARG	CA-CB-CG	5.37	125.22	113.40
1	S2	121	U	C6-N1-C2	-5.37	117.78	121.00
1	S2	176	C	C2-N3-C4	5.37	122.59	119.90
40	LA	1448	U	N3-C2-O2	-5.37	118.44	122.20
1	S2	489	C	C5-C6-N1	5.37	123.69	121.00
1	S2	352	A	P-O3'-C3'	5.37	126.14	119.70
1	S2	1632	C	N3-C2-O2	-5.37	118.14	121.90
40	LA	1614	C	C5-C6-N1	5.37	123.68	121.00
1	S2	1063	U	N3-C2-O2	-5.37	118.44	122.20
40	LA	829	U	C5-C6-N1	5.37	125.38	122.70
40	LA	2962	U	C5-C6-N1	5.37	125.38	122.70
40	LA	1208	U	N3-C2-O2	-5.36	118.45	122.20
36	Sm	67	C	N3-C2-O2	-5.35	118.15	121.90
1	S2	1699	G	C2-N3-C4	5.35	114.57	111.90
40	LA	1459	C	C6-N1-C2	-5.35	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1430	U	P-O3'-C3'	5.35	126.12	119.70
40	LA	217	U	OP1-P-O3'	5.35	116.97	105.20
40	LA	916	G	P-O3'-C3'	5.35	126.12	119.70
40	LA	1271	A	P-O3'-C3'	5.35	126.12	119.70
40	LA	2205	U	C2-N1-C1'	5.35	124.12	117.70
1	S2	911	U	N3-C2-O2	-5.34	118.46	122.20
25	Sb	126	LEU	CA-CB-CG	5.34	127.59	115.30
36	Sm	63	U	N3-C2-O2	-5.34	118.46	122.20
41	LB	44	C	C6-N1-C2	-5.34	118.16	120.30
40	LA	2681	U	C5-C6-N1	5.34	125.37	122.70
1	S2	440	U	C6-N1-C2	-5.34	117.80	121.00
40	LA	1276	U	C5-C6-N1	5.34	125.37	122.70
1	S2	820	U	N3-C2-O2	-5.34	118.46	122.20
40	LA	2330	C	C6-N1-C2	-5.33	118.17	120.30
37	Sn	63	G	P-O3'-C3'	5.33	126.10	119.70
42	LC	117	C	C6-N1-C2	-5.33	118.17	120.30
1	S2	1173	C	C6-N1-C2	-5.33	118.17	120.30
55	LP	113	LEU	CA-CB-CG	5.33	127.56	115.30
1	S2	1543	A	C2-N3-C4	5.33	113.26	110.60
40	LA	2983	C	N3-C2-O2	-5.33	118.17	121.90
1	S2	609	U	P-O3'-C3'	5.32	126.09	119.70
40	LA	860	G	N1-C6-O6	-5.32	116.71	119.90
40	LA	2929	C	C6-N1-C2	-5.32	118.17	120.30
40	LA	2742	C	C6-N1-C2	-5.32	118.17	120.30
11	SU	131	PHE	CB-CG-CD1	-5.32	117.08	120.80
40	LA	3233	C	C6-N1-C2	-5.32	118.17	120.30
40	LA	87	U	N3-C2-O2	-5.31	118.48	122.20
40	LA	1448	U	C5-C6-N1	5.31	125.36	122.70
40	LA	985	U	N3-C2-O2	-5.31	118.48	122.20
40	LA	609	G	OP2-P-O3'	5.31	116.88	105.20
40	LA	2298	U	C2-N1-C1'	5.31	124.07	117.70
40	LA	2836	C	O4'-C1'-N1	5.31	112.45	108.20
52	LM	28	ASP	CB-CG-OD1	5.31	123.08	118.30
40	LA	2825	C	N1-C2-O2	5.31	122.08	118.90
1	S2	90	C	C2-N1-C1'	5.30	124.64	118.80
1	S2	1528	U	C2-N1-C1'	5.30	124.06	117.70
1	S2	1799	U	C2-N1-C1'	5.30	124.07	117.70
36	Sm	62	C	O4'-C1'-N1	5.30	112.44	108.20
40	LA	915	A	C4-N9-C1'	5.30	135.85	126.30
40	LA	1759	C	C6-N1-C2	-5.30	118.18	120.30
1	S2	1075	C	C5-C6-N1	5.30	123.65	121.00
40	LA	225	C	C5-C6-N1	5.30	123.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	1685	C	C6-N1-C2	-5.30	118.18	120.30
1	S2	1115	U	C2-N1-C1'	5.30	124.06	117.70
40	LA	311	C	C6-N1-C2	-5.30	118.18	120.30
1	S2	921	U	C5-C6-N1	5.30	125.35	122.70
1	S2	627	C	N1-C2-O2	5.30	122.08	118.90
42	LC	127	U	C6-N1-C1'	-5.29	113.79	121.20
40	LA	860	G	C8-N9-C4	-5.29	104.28	106.40
40	LA	3058	U	C6-N1-C1'	-5.29	113.80	121.20
1	S2	1207	C	P-O3'-C3'	5.29	126.04	119.70
40	LA	282	G	P-O3'-C3'	5.28	126.04	119.70
1	S2	1045	C	C6-N1-C2	-5.28	118.19	120.30
40	LA	1722	U	N3-C2-O2	-5.28	118.50	122.20
40	LA	2899	C	O4'-C1'-N1	5.28	112.42	108.20
36	Sm	55	U	OP1-P-O3'	5.28	116.81	105.20
40	LA	3277	U	N1-C2-O2	5.28	126.50	122.80
36	Sm	70	C	C2-N1-C1'	5.28	124.60	118.80
40	LA	2359	C	C6-N1-C2	-5.28	118.19	120.30
1	S2	1347	U	N1-C2-O2	5.27	126.49	122.80
40	LA	1889	G	C8-N9-C1'	-5.27	120.15	127.00
40	LA	3349	C	C6-N1-C2	-5.27	118.19	120.30
1	S2	1739	C	C6-N1-C2	-5.27	118.19	120.30
40	LA	911	C	C5-C6-N1	5.27	123.63	121.00
1	S2	820	U	N1-C2-O2	5.26	126.48	122.80
1	S2	64	U	N3-C2-O2	-5.26	118.52	122.20
1	S2	629	U	N1-C2-O2	5.26	126.48	122.80
1	S2	886	U	C2-N1-C1'	5.26	124.01	117.70
1	S2	1332	C	C2-N1-C1'	5.26	124.58	118.80
37	Sn	72	U	C2-N1-C1'	5.26	124.01	117.70
1	S2	1012	U	C5-C4-O4	-5.26	122.75	125.90
40	LA	1275	C	C6-N1-C2	-5.25	118.20	120.30
40	LA	2496	C	N1-C2-O2	5.25	122.05	118.90
40	LA	1269	U	C6-N1-C1'	-5.25	113.84	121.20
40	LA	3214	U	C5-C6-N1	5.25	125.33	122.70
1	S2	1374	C	C5-C6-N1	5.25	123.63	121.00
40	LA	1064	A	OP2-P-O3'	5.25	116.75	105.20
1	S2	1620	C	C6-N1-C2	-5.25	118.20	120.30
1	S2	864	U	N1-C2-O2	5.25	126.47	122.80
40	LA	2760	C	C6-N1-C2	-5.25	118.20	120.30
1	S2	87	C	C6-N1-C2	-5.24	118.20	120.30
40	LA	354	U	C2-N1-C1'	5.24	123.99	117.70
40	LA	1779	C	C5-C6-N1	5.24	123.62	121.00
40	LA	2209	U	N3-C2-O2	-5.24	118.53	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	LB	78	U	N3-C2-O2	-5.24	118.53	122.20
1	S2	795	U	N1-C2-O2	5.24	126.46	122.80
40	LA	2836	C	C6-N1-C1'	-5.23	114.52	120.80
1	S2	1557	U	P-O3'-C3'	5.23	125.98	119.70
1	S2	1620	C	N3-C2-O2	-5.23	118.24	121.90
13	SW	150	LEU	CA-CB-CG	5.23	127.33	115.30
40	LA	524	U	N3-C2-O2	-5.23	118.54	122.20
46	LG	236	LEU	CA-CB-CG	5.23	127.33	115.30
40	LA	949	C	C6-N1-C2	-5.23	118.21	120.30
40	LA	977	C	C6-N1-C2	-5.23	118.21	120.30
40	LA	2366	C	C2-N1-C1'	5.23	124.55	118.80
84	Ls	114	LYS	CA-CB-CG	5.23	124.90	113.40
1	S2	912	U	P-O3'-C3'	5.23	125.97	119.70
1	S2	921	U	C2-N1-C1'	5.23	123.97	117.70
1	S2	656	G	C2-N3-C4	5.22	114.51	111.90
1	S2	1527	C	C6-N1-C1'	-5.22	114.53	120.80
1	S2	1202	A	C5-C6-N1	5.22	120.31	117.70
40	LA	2773	C	C2-N1-C1'	5.22	124.54	118.80
40	LA	3306	U	O4'-C1'-N1	5.22	112.38	108.20
1	S2	476	U	OP1-P-O3'	5.22	116.68	105.20
40	LA	2098	C	C5-C6-N1	5.22	123.61	121.00
36	Sm	62	C	N1-C2-N3	5.22	122.85	119.20
1	S2	795	U	C2-N1-C1'	5.22	123.96	117.70
1	S2	68	A	C8-N9-C4	-5.21	103.72	105.80
40	LA	1822	C	C6-N1-C2	-5.21	118.22	120.30
40	LA	2411	U	N3-C2-O2	-5.21	118.55	122.20
42	LC	127	U	C5-C6-N1	5.21	125.31	122.70
40	LA	2340	U	C5-C6-N1	5.21	125.30	122.70
40	LA	868	C	C6-N1-C2	-5.20	118.22	120.30
40	LA	1230	G	N1-C2-N2	-5.20	111.52	116.20
40	LA	2570	U	N1-C2-O2	5.20	126.44	122.80
40	LA	1155	C	C5-C6-N1	5.20	123.60	121.00
40	LA	2505	U	N1-C2-O2	5.20	126.44	122.80
40	LA	427	C	C6-N1-C2	-5.20	118.22	120.30
40	LA	2541	U	C2-N1-C1'	5.20	123.94	117.70
40	LA	2925	C	N1-C2-O2	5.20	122.02	118.90
1	S2	587	C	C6-N1-C2	-5.20	118.22	120.30
40	LA	2842	U	N3-C2-O2	-5.20	118.56	122.20
1	S2	1274	C	C2-N1-C1'	5.20	124.52	118.80
1	S2	1639	C	C6-N1-C2	-5.20	118.22	120.30
36	Sm	49	G	C2-N3-C4	5.20	114.50	111.90
40	LA	650	C	C6-N1-C2	-5.20	118.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	777	U	N3-C2-O2	-5.19	118.56	122.20
40	LA	855	U	N3-C2-O2	-5.19	118.57	122.20
40	LA	1269	U	C5-C6-N1	5.19	125.30	122.70
40	LA	2925	C	N3-C2-O2	-5.19	118.27	121.90
40	LA	3105	U	N3-C2-O2	-5.19	118.57	122.20
1	S2	1066	C	C2-N1-C1'	5.19	124.51	118.80
40	LA	375	A	OP1-P-O3'	5.18	116.61	105.20
40	LA	1052	U	N3-C2-O2	-5.18	118.57	122.20
40	LA	1563	C	O4'-C1'-N1	5.18	112.35	108.20
40	LA	2620	G	N1-C6-O6	-5.18	116.79	119.90
1	S2	185	U	O5'-P-OP2	-5.18	101.04	105.70
1	S2	453	U	C2-N1-C1'	5.18	123.92	117.70
40	LA	2133	U	N3-C2-O2	-5.18	118.57	122.20
40	LA	1756	C	C6-N1-C2	-5.18	118.23	120.30
36	Sm	7	U	C6-N1-C1'	-5.18	113.95	121.20
37	Sn	56	C	C6-N1-C2	-5.18	118.23	120.30
40	LA	3121	U	OP1-P-O3'	5.18	116.59	105.20
1	S2	911	U	C2-N1-C1'	5.17	123.91	117.70
40	LA	1368	U	C5-C6-N1	5.17	125.29	122.70
1	S2	886	U	C5-C6-N1	5.17	125.29	122.70
26	Sc	104	LEU	CA-CB-CG	5.17	127.20	115.30
40	LA	637	C	OP1-P-O3'	5.17	116.57	105.20
40	LA	2689	A	C2-N3-C4	5.17	113.18	110.60
1	S2	1573	A	OP2-P-O3'	5.16	116.56	105.20
40	LA	743	C	N1-C2-O2	5.16	122.00	118.90
1	S2	1535	U	C2-N1-C1'	5.16	123.89	117.70
27	Sd	74	LEU	CB-CG-CD2	-5.16	102.23	111.00
40	LA	1706	C	N3-C2-O2	-5.16	118.29	121.90
40	LA	982	C	C6-N1-C2	-5.16	118.24	120.30
1	S2	442	C	C6-N1-C2	-5.16	118.24	120.30
1	S2	1066	C	N1-C2-O2	5.16	121.99	118.90
1	S2	1497	U	C5-C6-N1	5.16	125.28	122.70
40	LA	2194	G	N3-C4-C5	-5.16	126.02	128.60
40	LA	3319	U	P-O3'-C3'	5.16	125.89	119.70
1	S2	302	U	N3-C2-O2	-5.15	118.59	122.20
1	S2	1121	C	C6-N1-C2	-5.15	118.24	120.30
40	LA	142	C	C5-C6-N1	5.15	123.58	121.00
84	Ls	6	HIS	C-N-CA	5.15	134.57	121.70
36	Sm	34	U	C5-C6-N1	5.15	125.27	122.70
37	Sn	25	C	C5-C6-N1	5.15	123.57	121.00
1	S2	1023	A	P-O3'-C3'	5.14	125.87	119.70
40	LA	3298	C	C6-N1-C2	-5.14	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	608	U	O4'-C1'-N1	5.14	112.31	108.20
40	LA	492	C	N3-C2-O2	-5.14	118.30	121.90
13	SW	99	LEU	CA-CB-CG	5.14	127.12	115.30
40	LA	873	C	P-O3'-C3'	5.14	125.86	119.70
40	LA	979	U	C2-N1-C1'	5.14	123.86	117.70
40	LA	609	G	N3-C4-N9	5.13	129.08	126.00
1	S2	897	C	C6-N1-C2	-5.13	118.25	120.30
84	Ls	32	VAL	CA-CB-CG1	5.13	118.59	110.90
40	LA	1764	U	OP1-P-O3'	5.13	116.48	105.20
1	S2	1709	C	N1-C2-O2	5.12	121.97	118.90
42	LC	21	C	C6-N1-C1'	-5.12	114.65	120.80
1	S2	1332	C	C6-N1-C2	-5.12	118.25	120.30
40	LA	2350	C	C6-N1-C2	-5.12	118.25	120.30
1	S2	387	A	OP2-P-O3'	5.12	116.46	105.20
40	LA	1358	C	C6-N1-C2	-5.12	118.25	120.30
40	LA	2151	C	C6-N1-C2	-5.12	118.25	120.30
3	SP	9	LEU	CA-CB-CG	5.12	127.07	115.30
84	Ls	102	LEU	CB-CG-CD2	5.12	119.70	111.00
11	SU	64	VAL	CA-CB-CG1	5.11	118.57	110.90
36	Sm	11	C	C6-N1-C2	-5.11	118.25	120.30
1	S2	224	C	OP1-P-O3'	5.11	116.44	105.20
41	LB	28	C	N3-C2-O2	-5.11	118.32	121.90
40	LA	3206	C	C6-N1-C2	-5.11	118.26	120.30
40	LA	113	C	C6-N1-C2	-5.11	118.26	120.30
40	LA	621	A	C2-N3-C4	5.11	113.15	110.60
40	LA	2553	U	C2-N1-C1'	5.11	123.83	117.70
1	S2	1404	C	C6-N1-C2	-5.11	118.26	120.30
1	S2	1699	G	N3-C4-C5	-5.11	126.05	128.60
36	Sm	60	U	C6-N1-C1'	-5.11	114.05	121.20
40	LA	1276	U	N3-C2-O2	-5.11	118.63	122.20
40	LA	548	G	C6-N1-C2	-5.10	122.04	125.10
40	LA	2277	C	C5-C6-N1	5.10	123.55	121.00
41	LB	40	C	N1-C2-O2	5.10	121.96	118.90
1	S2	1012	U	N1-C2-O2	5.10	126.37	122.80
1	S2	1491	U	N1-C2-O2	5.10	126.37	122.80
40	LA	2189	U	C2-N1-C1'	5.10	123.82	117.70
42	LC	30	C	C6-N1-C2	-5.09	118.26	120.30
40	LA	922	U	C5-C6-N1	5.09	125.25	122.70
1	S2	250	C	C6-N1-C2	-5.09	118.26	120.30
1	S2	758	U	C2-N1-C1'	5.09	123.81	117.70
40	LA	1843	C	C6-N1-C2	-5.09	118.26	120.30
40	LA	2550	U	N1-C2-O2	5.09	126.36	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	817	A	C8-N9-C4	-5.09	103.77	105.80
41	LB	35	C	C6-N1-C2	-5.09	118.27	120.30
36	Sm	53	G	N1-C2-N2	-5.09	111.62	116.20
1	S2	1414	U	N1-C2-O2	5.08	126.36	122.80
1	S2	121	U	N1-C2-O2	5.08	126.36	122.80
40	LA	982	C	C5-C6-N1	5.08	123.54	121.00
47	LH	142	ASP	CB-CG-OD1	5.08	122.87	118.30
1	S2	1080	U	C2-N1-C1'	5.08	123.80	117.70
1	S2	1145	U	C6-N1-C1'	-5.08	114.09	121.20
1	S2	1258	U	C6-N1-C1'	-5.08	114.09	121.20
42	LC	71	A	O4'-C1'-N9	-5.08	104.14	108.20
40	LA	544	C	N1-C2-O2	5.08	121.95	118.90
40	LA	1446	A	O5'-P-OP1	-5.08	101.13	105.70
1	S2	1082	C	N3-C2-O2	-5.08	118.35	121.90
40	LA	1037	C	C5-C6-N1	5.08	123.54	121.00
1	S2	499	U	C6-N1-C2	-5.07	117.96	121.00
40	LA	3174	A	O4'-C1'-N9	5.07	112.26	108.20
1	S2	1342	C	N1-C2-O2	5.07	121.94	118.90
1	S2	1485	C	N1-C2-O2	5.07	121.94	118.90
40	LA	2102	U	C6-N1-C2	-5.07	117.96	121.00
1	S2	1571	C	C6-N1-C2	-5.07	118.27	120.30
1	S2	1674	C	C5-C6-N1	5.07	123.53	121.00
40	LA	1540	U	N3-C2-O2	-5.07	118.65	122.20
40	LA	800	G	C4-N9-C1'	5.06	133.08	126.50
40	LA	3089	C	C5-C6-N1	5.06	123.53	121.00
40	LA	224	C	C6-N1-C2	-5.06	118.28	120.30
40	LA	1779	C	C6-N1-C2	-5.06	118.28	120.30
1	S2	950	C	C6-N1-C2	-5.06	118.28	120.30
40	LA	1832	C	C6-N1-C2	-5.06	118.28	120.30
40	LA	3269	U	C6-N1-C1'	-5.06	114.12	121.20
40	LA	954	U	N3-C2-O2	-5.05	118.66	122.20
1	S2	1491	U	N3-C2-O2	-5.05	118.66	122.20
17	SY	137	PRO	C-N-CA	5.05	134.33	121.70
40	LA	524	U	C2-N1-C1'	5.05	123.76	117.70
40	LA	1470	U	N1-C2-O2	5.05	126.33	122.80
40	LA	3120	C	C6-N1-C2	-5.05	118.28	120.30
1	S2	804	A	N7-C8-N9	5.05	116.32	113.80
40	LA	2712	U	N3-C2-O2	-5.05	118.67	122.20
5	SE	25	LEU	CA-CB-CG	5.05	126.91	115.30
40	LA	1943	C	C5-C6-N1	5.05	123.52	121.00
40	LA	1496	C	C6-N1-C1'	-5.04	114.75	120.80
1	S2	583	C	C6-N1-C1'	-5.04	114.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	LA	1276	U	C6-N1-C2	-5.04	117.97	121.00
40	LA	1296	C	C6-N1-C2	-5.04	118.28	120.30
40	LA	315	C	C6-N1-C2	-5.04	118.28	120.30
1	S2	1067	C	C6-N1-C2	-5.04	118.28	120.30
40	LA	2257	C	C5-C6-N1	5.04	123.52	121.00
1	S2	35	U	N1-C2-O2	5.04	126.33	122.80
1	S2	1285	U	N3-C4-O4	-5.04	115.87	119.40
40	LA	2495	C	C5-C6-N1	5.04	123.52	121.00
1	S2	184	C	C2-N1-C1'	5.04	124.34	118.80
40	LA	2594	C	C6-N1-C2	-5.04	118.29	120.30
84	Ls	32	VAL	CG1-CB-CG2	-5.03	102.85	110.90
1	S2	1458	G	OP2-P-O3'	5.03	116.27	105.20
1	S2	1186	U	C5-C6-N1	5.03	125.21	122.70
40	LA	803	C	C5-C6-N1	5.03	123.51	121.00
40	LA	2617	U	C2-N1-C1'	5.02	123.73	117.70
40	LA	2684	C	C6-N1-C2	-5.02	118.29	120.30
37	Sn	69	C	C6-N1-C2	-5.02	118.29	120.30
40	LA	1556	C	C2-N1-C1'	5.02	124.32	118.80
40	LA	2585	G	C2-N3-C4	5.02	114.41	111.90
51	LL	212	GLU	C-N-CA	5.02	134.24	121.70
53	LN	22	VAL	CG1-CB-CG2	-5.01	102.88	110.90
40	LA	2209	U	N1-C2-O2	5.01	126.31	122.80
40	LA	2552	C	N3-C2-O2	-5.01	118.39	121.90
40	LA	2963	C	C6-N1-C2	-5.01	118.30	120.30
1	S2	583	C	N3-C2-O2	-5.01	118.39	121.90
40	LA	179	C	C6-N1-C2	-5.01	118.30	120.30
40	LA	2132	C	N1-C2-O2	5.01	121.91	118.90
40	LA	439	C	C6-N1-C2	-5.01	118.30	120.30
40	LA	800	G	C2-N3-C4	5.01	114.41	111.90
40	LA	2388	U	N1-C2-O2	5.01	126.31	122.80
40	LA	3105	U	N1-C2-O2	5.01	126.31	122.80
1	S2	1214	U	C2-N1-C1'	5.01	123.71	117.70
40	LA	979	U	N1-C2-O2	5.00	126.30	122.80
40	LA	1525	G	C4-N9-C1'	5.00	133.00	126.50
40	LA	3355	U	N1-C2-O2	5.00	126.30	122.80
41	LB	39	C	C5-C6-N1	5.00	123.50	121.00
42	LC	72	A	O5'-P-OP2	-5.00	101.20	105.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
84	Ls	51	5CT	C2

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
86	A	1198	SER	Peptide
86	A	1256	LEU	Mainchain
86	A	1340	LYS	Mainchain
86	A	1580	ALA	Peptide
86	A	1615	ALA	Mainchain
86	A	1639	ALA	Peptide
86	A	1705	ALA	Peptide
86	A	1819	ALA	Mainchain
86	A	2019	ALA	Mainchain
86	A	2330	ALA	Mainchain
86	A	950	ALA	Mainchain
86	A	982	ALA	Peptide
45	LF	13	GLY	Peptide
45	LF	3	ARG	Peptide
45	LF	318	LEU	Peptide
48	LI	232	ARG	Peptide
49	LJ	30	THR	Peptide
49	LJ	76	ALA	Peptide
49	LJ	77	GLN	Peptide
58	LS	161	LYS	Peptide
68	Lc	115	LYS	Peptide
68	Lc	14	HIS	Peptide
69	Ld	19	ASN	Peptide
69	Ld	20	GLY	Peptide
70	Le	47	ASN	Peptide
71	Lf	7	VAL	Peptide
75	Lj	83	LYS	Peptide
84	Ls	112	ASP	Peptide
84	Ls	97	ASP	Peptide
85	Lt	191	UNK	Peptide
85	Lt	192	UNK	Peptide
85	Lt	203	UNK	Peptide
85	Lt	56	UNK	Peptide
9	SB	125	THR	Peptide
9	SB	42	LEU	Peptide
16	SD	108	ARG	Peptide
19	SF	40	GLU	Peptide
22	SI	120	GLY	Peptide
33	SN	147	VAL	Peptide
8	SS	193	GLY	Peptide
11	SU	64	VAL	Peptide
18	SZ	90	ARG	Peptide

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Mol	Chain	Res	Type	Group
25	Sb	54	ASP	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	SP	204/206 (99%)	183 (90%)	21 (10%)	0	100	100
4	SQ	222/232 (96%)	201 (90%)	21 (10%)	0	100	100
5	SE	115/117 (98%)	100 (87%)	15 (13%)	0	100	100
6	SR	214/216 (99%)	190 (89%)	24 (11%)	0	100	100
7	SA	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
8	SS	256/258 (99%)	229 (90%)	27 (10%)	0	100	100
9	SB	204/206 (99%)	189 (93%)	15 (7%)	0	100	100
10	ST	226/228 (99%)	211 (93%)	14 (6%)	1 (0%)	30	65
11	SU	182/184 (99%)	163 (90%)	19 (10%)	0	100	100
12	SV	183/198 (92%)	167 (91%)	16 (9%)	0	100	100
13	SW	182/184 (99%)	165 (91%)	16 (9%)	1 (0%)	25	60
14	SC	90/92 (98%)	79 (88%)	11 (12%)	0	100	100
15	SX	140/142 (99%)	124 (89%)	16 (11%)	0	100	100
16	SD	119/121 (98%)	91 (76%)	26 (22%)	2 (2%)	7	36
17	SY	148/150 (99%)	133 (90%)	15 (10%)	0	100	100
18	SZ	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
19	SF	139/141 (99%)	125 (90%)	14 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	SG	117/125 (94%)	112 (96%)	5 (4%)	0	100	100
21	SH	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
22	SI	141/143 (99%)	128 (91%)	13 (9%)	0	100	100
23	SJ	98/100 (98%)	88 (90%)	10 (10%)	0	100	100
24	Sa	85/87 (98%)	73 (86%)	12 (14%)	0	100	100
25	Sb	127/129 (98%)	113 (89%)	14 (11%)	0	100	100
26	Sc	142/144 (99%)	123 (87%)	19 (13%)	0	100	100
27	Sd	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
28	SK	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
29	Se	95/97 (98%)	84 (88%)	11 (12%)	0	100	100
30	Sf	79/81 (98%)	67 (85%)	12 (15%)	0	100	100
31	SM	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
32	Sg	55/57 (96%)	43 (78%)	12 (22%)	0	100	100
33	SN	71/73 (97%)	48 (68%)	23 (32%)	0	100	100
34	SO	310/312 (99%)	268 (86%)	42 (14%)	0	100	100
35	SL	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
38	So	341/366 (93%)	311 (91%)	30 (9%)	0	100	100
43	LD	249/251 (99%)	223 (90%)	26 (10%)	0	100	100
44	LE	384/386 (100%)	355 (92%)	29 (8%)	0	100	100
45	LF	359/361 (99%)	323 (90%)	35 (10%)	1 (0%)	37	70
46	LG	292/294 (99%)	266 (91%)	26 (9%)	0	100	100
47	LH	163/175 (93%)	147 (90%)	16 (10%)	0	100	100
48	LI	220/222 (99%)	203 (92%)	17 (8%)	0	100	100
49	LJ	231/233 (99%)	208 (90%)	23 (10%)	0	100	100
50	LK	189/191 (99%)	174 (92%)	15 (8%)	0	100	100
51	LL	216/218 (99%)	189 (88%)	27 (12%)	0	100	100
52	LM	167/169 (99%)	153 (92%)	14 (8%)	0	100	100
53	LN	191/193 (99%)	171 (90%)	19 (10%)	1 (0%)	25	60
54	LO	134/136 (98%)	121 (90%)	13 (10%)	0	100	100
55	LP	201/203 (99%)	181 (90%)	19 (10%)	1 (0%)	25	60
56	LQ	195/197 (99%)	186 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	LR	181/183 (99%)	168 (93%)	13 (7%)	0	100	100
58	LS	183/185 (99%)	170 (93%)	13 (7%)	0	100	100
59	LT	186/188 (99%)	178 (96%)	8 (4%)	0	100	100
60	LU	169/171 (99%)	159 (94%)	10 (6%)	0	100	100
61	LV	157/159 (99%)	143 (91%)	14 (9%)	0	100	100
62	LW	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
63	LX	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
64	LY	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
65	LZ	119/121 (98%)	110 (92%)	9 (8%)	0	100	100
66	La	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
67	Lb	133/135 (98%)	117 (88%)	16 (12%)	0	100	100
68	Lc	146/148 (99%)	130 (89%)	16 (11%)	0	100	100
69	Ld	56/58 (97%)	47 (84%)	9 (16%)	0	100	100
70	Le	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
71	Lf	107/109 (98%)	93 (87%)	14 (13%)	0	100	100
72	Lg	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
73	Lh	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
74	Li	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
75	Lj	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
76	Lk	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
77	Ll	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
78	Lm	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
79	Ln	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
80	Lo	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
81	Lp	23/25 (92%)	23 (100%)	0	0	100	100
82	Lq	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
83	Lr	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
84	Ls	151/154 (98%)	117 (78%)	31 (20%)	3 (2%)	6	33
86	A	1182/1209 (98%)	929 (79%)	190 (16%)	63 (5%)	1	18
All	All	12588/12828 (98%)	11260 (90%)	1255 (10%)	73 (1%)	24	57

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
84	Ls	133	ASP
86	A	1162	ALA
86	A	1163	LEU
86	A	1164	SER
86	A	1182	PRO
86	A	1341	TYR
86	A	1353	GLN
86	A	1394	ILE
86	A	1421	PRO
86	A	1442	ALA
86	A	1459	ALA
86	A	1538	ALA
86	A	1541	ALA
86	A	1561	ALA
86	A	1616	ALA
86	A	1820	ALA
86	A	1832	ALA
86	A	1839	ALA
86	A	1900	ALA
86	A	2020	ALA
86	A	2032	ALA
86	A	2039	ALA
86	A	2101	ALA
86	A	2232	ALA
86	A	2239	ALA
86	A	2300	ALA
86	A	2331	ALA
86	A	2343	ALA
86	A	2350	ALA
86	A	2411	ALA
16	SD	109	GLU
86	A	1136	ASN
86	A	1245	VAL
86	A	1249	ILE
86	A	1257	ASP
86	A	1290	VAL
86	A	1691	ALA
86	A	1815	ALA
86	A	1873	ALA
86	A	2015	ALA
86	A	2073	ALA
86	A	2273	ALA
86	A	2326	ALA

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Mol	Chain	Res	Type
86	A	2384	ALA
45	LF	4	PRO
84	Ls	8	PHE
86	A	1402	ILE
86	A	1454	ALA
86	A	1457	ALA
86	A	1521	ALA
86	A	1618	ALA
86	A	1707	ALA
86	A	1881	ALA
86	A	2081	ALA
86	A	2281	ALA
86	A	2392	ALA
84	Ls	98	GLY
86	A	943	ALA
86	A	1137	PRO
86	A	1277	LEU
86	A	1537	ALA
86	A	1556	ALA
86	A	1600	ALA
86	A	1637	ALA
86	A	1223	PRO
86	A	1641	ALA
55	LP	146	ALA
86	A	1236	ILE
13	SW	18	PRO
53	LN	61	PRO
10	ST	226	ILE
16	SD	127	GLY
86	A	1338	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	SP	170/173 (98%)	169 (99%)	1 (1%)	84 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	SQ	200/205 (98%)	199 (100%)	1 (0%)	86	90
5	SE	95/98 (97%)	95 (100%)	0	100	100
6	SR	175/175 (100%)	175 (100%)	0	100	100
7	SA	182/182 (100%)	180 (99%)	2 (1%)	70	79
8	SS	220/220 (100%)	218 (99%)	2 (1%)	75	83
9	SB	172/173 (99%)	172 (100%)	0	100	100
10	ST	189/195 (97%)	186 (98%)	3 (2%)	58	73
11	SU	163/165 (99%)	163 (100%)	0	100	100
12	SV	148/159 (93%)	148 (100%)	0	100	100
13	SW	156/157 (99%)	153 (98%)	3 (2%)	52	70
14	SC	77/85 (91%)	76 (99%)	1 (1%)	65	76
15	SX	126/127 (99%)	124 (98%)	2 (2%)	58	73
16	SD	88/98 (90%)	88 (100%)	0	100	100
17	SY	127/127 (100%)	126 (99%)	1 (1%)	79	84
18	SZ	90/96 (94%)	89 (99%)	1 (1%)	70	79
19	SF	117/117 (100%)	116 (99%)	1 (1%)	75	83
20	SG	101/113 (89%)	101 (100%)	0	100	100
21	SH	127/128 (99%)	125 (98%)	2 (2%)	58	73
22	SI	115/115 (100%)	115 (100%)	0	100	100
23	SJ	93/93 (100%)	92 (99%)	1 (1%)	70	79
24	Sa	71/74 (96%)	71 (100%)	0	100	100
25	Sb	110/110 (100%)	110 (100%)	0	100	100
26	Sc	119/119 (100%)	119 (100%)	0	100	100
27	Sd	102/112 (91%)	101 (99%)	1 (1%)	73	81
28	SK	67/73 (92%)	66 (98%)	1 (2%)	60	74
29	Se	82/83 (99%)	82 (100%)	0	100	100
30	Sf	70/70 (100%)	69 (99%)	1 (1%)	62	75
31	SM	47/47 (100%)	47 (100%)	0	100	100
32	Sg	48/49 (98%)	48 (100%)	0	100	100
33	SN	56/63 (89%)	56 (100%)	0	100	100
34	SO	250/257 (97%)	250 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	SL	55/56 (98%)	55 (100%)	0	100	100
38	So	298/308 (97%)	298 (100%)	0	100	100
43	LD	190/193 (98%)	189 (100%)	1 (0%)	86	90
44	LE	318/322 (99%)	317 (100%)	1 (0%)	91	92
45	LF	288/288 (100%)	287 (100%)	1 (0%)	91	92
46	LG	241/243 (99%)	241 (100%)	0	100	100
47	LH	139/154 (90%)	139 (100%)	0	100	100
48	LI	186/186 (100%)	186 (100%)	0	100	100
49	LJ	187/191 (98%)	186 (100%)	1 (0%)	86	90
50	LK	168/171 (98%)	167 (99%)	1 (1%)	84	88
51	LL	185/185 (100%)	183 (99%)	2 (1%)	70	79
52	LM	145/147 (99%)	144 (99%)	1 (1%)	81	86
53	LN	154/154 (100%)	152 (99%)	2 (1%)	65	76
54	LO	107/107 (100%)	107 (100%)	0	100	100
55	LP	175/175 (100%)	175 (100%)	0	100	100
56	LQ	160/160 (100%)	160 (100%)	0	100	100
57	LR	138/145 (95%)	138 (100%)	0	100	100
58	LS	150/150 (100%)	146 (97%)	4 (3%)	40	60
59	LT	152/153 (99%)	148 (97%)	4 (3%)	41	61
60	LU	155/155 (100%)	155 (100%)	0	100	100
61	LV	135/136 (99%)	133 (98%)	2 (2%)	60	74
62	LW	87/87 (100%)	87 (100%)	0	100	100
63	LX	104/104 (100%)	104 (100%)	0	100	100
64	LY	54/57 (95%)	54 (100%)	0	100	100
65	LZ	104/105 (99%)	104 (100%)	0	100	100
66	La	108/108 (100%)	106 (98%)	2 (2%)	52	70
67	Lb	112/115 (97%)	111 (99%)	1 (1%)	75	83
68	Lc	117/118 (99%)	115 (98%)	2 (2%)	56	72
69	Ld	46/46 (100%)	45 (98%)	1 (2%)	47	65
70	Le	81/81 (100%)	79 (98%)	2 (2%)	42	62
71	Lf	92/96 (96%)	91 (99%)	1 (1%)	70	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	Lg	108/109 (99%)	107 (99%)	1 (1%)	75	83
73	Lh	90/90 (100%)	89 (99%)	1 (1%)	70	79
74	Li	95/95 (100%)	95 (100%)	0	100	100
75	Lj	104/104 (100%)	102 (98%)	2 (2%)	52	70
76	Lk	80/81 (99%)	79 (99%)	1 (1%)	65	76
77	Ll	67/67 (100%)	64 (96%)	3 (4%)	23	48
78	Lm	68/68 (100%)	68 (100%)	0	100	100
79	Ln	45/45 (100%)	45 (100%)	0	100	100
80	Lo	45/47 (96%)	44 (98%)	1 (2%)	47	65
81	Lp	22/23 (96%)	22 (100%)	0	100	100
82	Lq	87/88 (99%)	86 (99%)	1 (1%)	70	79
83	Lr	71/71 (100%)	66 (93%)	5 (7%)	12	36
84	Ls	118/129 (92%)	116 (98%)	2 (2%)	56	72
All	All	9584/9771 (98%)	9514 (99%)	70 (1%)	80	86

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	SP	39	ASN
4	SQ	7	LYS
7	SA	76	ARG
7	SA	185	LYS
8	SS	96	ASN
8	SS	211	LYS
10	ST	46	LYS
10	ST	143	LYS
10	ST	214	LYS
13	SW	39	LYS
13	SW	132	ARG
13	SW	149	ARG
14	SC	64	TYR
15	SX	32	LYS
15	SX	67	ARG
17	SY	64	ARG
18	SZ	136	ARG
19	SF	107	LYS
21	SH	98	TYR

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Mol	Chain	Res	Type
21	SH	145	ARG
23	SJ	43	LYS
27	Sd	111	LYS
28	SK	85	LYS
30	Sf	36	LYS
43	LD	242	ARG
44	LE	332	ARG
45	LF	98	ARG
49	LJ	213	LYS
50	LK	59	ASN
51	LL	185	ARG
51	LL	208	ASN
52	LM	85	LYS
53	LN	31	LYS
53	LN	104	ARG
58	LS	12	ARG
58	LS	31	LYS
58	LS	151	ARG
58	LS	159	LYS
59	LT	3	ASN
59	LT	81	ARG
59	LT	165	LYS
59	LT	166	ASN
61	LV	10	ARG
61	LV	83	ARG
66	La	74	TYR
66	La	108	LYS
67	Lb	3	LYS
68	Lc	77	LYS
68	Lc	92	LYS
69	Ld	33	LYS
70	Le	35	ARG
70	Le	83	LYS
71	Lf	87	ASN
72	Lg	8	LYS
73	Lh	73	ARG
75	Lj	10	ARG
75	Lj	59	ASN
76	Lk	4	LYS
77	Ll	11	ARG
77	Ll	19	CYS
77	Ll	22	CYS

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Mol	Chain	Res	Type
80	Lo	112	LYS
82	Lq	78	LYS
83	Lr	4	ARG
83	Lr	45	LYS
83	Lr	57	CYS
83	Lr	62	LYS
83	Lr	85	ARG
84	Ls	87	ARG
84	Ls	102	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
3	SP	39	ASN
8	SS	36	HIS
8	SS	69	HIS
8	SS	96	ASN
9	SB	100	ASN
9	SB	103	ASN
10	ST	56	ASN
10	ST	59	GLN
10	ST	139	ASN
10	ST	189	HIS
10	ST	190	GLN
10	ST	201	GLN
12	SV	20	GLN
12	SV	103	GLN
13	SW	112	GLN
14	SC	62	GLN
14	SC	81	ASN
17	SY	58	HIS
19	SF	77	GLN
21	SH	19	ASN
21	SH	122	HIS
22	SI	138	GLN
23	SJ	49	ASN
25	Sb	80	ASN
27	Sd	34	ASN
27	Sd	77	ASN
27	Sd	110	GLN
29	Se	43	ASN
33	SN	123	ASN

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Mol	Chain	Res	Type
33	SN	145	HIS
33	SN	151	ASN
34	SO	159	ASN
38	So	292	GLN
43	LD	47	GLN
43	LD	97	ASN
44	LE	139	GLN
44	LE	273	HIS
44	LE	279	ASN
45	LF	296	GLN
45	LF	322	GLN
46	LG	206	GLN
49	LJ	59	GLN
49	LJ	77	GLN
50	LK	59	ASN
50	LK	157	ASN
53	LN	19	GLN
53	LN	25	HIS
54	LO	41	GLN
55	LP	117	ASN
55	LP	182	ASN
56	LQ	55[A]	HIS
57	LR	97	ASN
58	LS	45	ASN
59	LT	3	ASN
59	LT	166	ASN
68	Lc	64	GLN
70	Le	75	ASN
71	Lf	87	ASN
73	Lh	42	GLN
74	Li	52	GLN
74	Li	61	GLN
76	Lk	92	ASN
79	Ln	25	GLN
82	Lq	23	HIS
82	Lq	59	HIS
84	Ls	88	ASN

### 5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1768/1800 (98%)	533 (30%)	52 (2%)
2	Sl	5/6 (83%)	1 (20%)	0
36	Sm	75/76 (98%)	35 (46%)	0
37	Sn	74/75 (98%)	23 (31%)	0
40	LA	3180/3394 (93%)	716 (22%)	42 (1%)
41	LB	120/121 (99%)	15 (12%)	1 (0%)
42	LC	157/158 (99%)	32 (20%)	3 (1%)
All	All	5379/5630 (95%)	1355 (25%)	98 (1%)

All (1355) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	4	C
1	S2	14	C
1	S2	25	C
1	S2	26	A
1	S2	34	G
1	S2	43	A
1	S2	45	U
1	S2	47	A
1	S2	56	U
1	S2	57	G
1	S2	62	A
1	S2	65	A
1	S2	67	A
1	S2	68	A
1	S2	69	G
1	S2	73	U
1	S2	74	U
1	S2	75	U
1	S2	76	A
1	S2	78	A
1	S2	79	C
1	S2	80	A
1	S2	81	G
1	S2	104	A
1	S2	114	C
1	S2	116	U
1	S2	121	U
1	S2	127	G

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Mol	Chain	Res	Type
1	S2	129	U
1	S2	130	C
1	S2	131	C
1	S2	132	U
1	S2	133	U
1	S2	134	U
1	S2	135	A
1	S2	136	C
1	S2	137	U
1	S2	138	A
1	S2	140	A
1	S2	141	U
1	S2	142	G
1	S2	153	G
1	S2	155	U
1	S2	156	A
1	S2	158	U
1	S2	161	U
1	S2	168	A
1	S2	171	A
1	S2	172	C
1	S2	174	U
1	S2	176	C
1	S2	178	U
1	S2	179	A
1	S2	182	A
1	S2	185	U
1	S2	186	C
1	S2	187	G
1	S2	188	A
1	S2	189	C
1	S2	191	C
1	S2	193	U
1	S2	194	U
1	S2	195	G
1	S2	201	G
1	S2	203	U
1	S2	204	G
1	S2	216	U
1	S2	217	A
1	S2	218	A
1	S2	223	U

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Mol	Chain	Res	Type
1	S2	224	C
1	S2	225	A
1	S2	227	U
1	S2	228	G
1	S2	230	C
1	S2	232	U
1	S2	233	C
1	S2	234	G
1	S2	235	G
1	S2	236	A
1	S2	238	U
1	S2	240	U
1	S2	241	U
1	S2	243	G
1	S2	246	G
1	S2	250	C
1	S2	256	A
1	S2	260	U
1	S2	261	U
1	S2	265	A
1	S2	270	C
1	S2	272	U
1	S2	274	G
1	S2	276	C
1	S2	277	U
1	S2	278	U
1	S2	279	G
1	S2	280	U
1	S2	287	G
1	S2	299	A
1	S2	313	U
1	S2	314	C
1	S2	316	A
1	S2	320	U
1	S2	321	C
1	S2	322	G
1	S2	323	A
1	S2	324	U
1	S2	330	G
1	S2	333	A
1	S2	334	G
1	S2	337	G

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Mol	Chain	Res	Type
1	S2	338	C
1	S2	352	A
1	S2	353	A
1	S2	359	A
1	S2	360	A
1	S2	361	C
1	S2	369	A
1	S2	370	A
1	S2	373	G
1	S2	378	A
1	S2	380	U
1	S2	388	G
1	S2	390	G
1	S2	400	A
1	S2	401	A
1	S2	402	C
1	S2	404	G
1	S2	406	U
1	S2	411	C
1	S2	415	C
1	S2	417	A
1	S2	419	G
1	S2	423	G
1	S2	424	C
1	S2	425	A
1	S2	426	G
1	S2	434	G
1	S2	435	C
1	S2	438	A
1	S2	439	U
1	S2	444	C
1	S2	446	A
1	S2	447	U
1	S2	448	C
1	S2	454	U
1	S2	460	A
1	S2	468	A
1	S2	482	U
1	S2	485	A
1	S2	487	G
1	S2	489	C
1	S2	491	C

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Mol	Chain	Res	Type
1	S2	492	A
1	S2	493	U
1	S2	494	U
1	S2	495	C
1	S2	496	G
1	S2	498	G
1	S2	499	U
1	S2	500	C
1	S2	502	U
1	S2	506	A
1	S2	507	U
1	S2	510	G
1	S2	511	A
1	S2	512	A
1	S2	513	U
1	S2	517	U
1	S2	518	A
1	S2	519	C
1	S2	520	A
1	S2	525	A
1	S2	527	A
1	S2	529	A
1	S2	534	A
1	S2	538	A
1	S2	539	G
1	S2	540	G
1	S2	541	A
1	S2	542	A
1	S2	543	C
1	S2	554	C
1	S2	555	A
1	S2	556	A
1	S2	557	G
1	S2	558	U
1	S2	565	C
1	S2	571	G
1	S2	572	C
1	S2	578	U
1	S2	579	A
1	S2	580	A
1	S2	594	A
1	S2	595	G

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Mol	Chain	Res	Type
1	S2	606	A
1	S2	609	U
1	S2	610	G
1	S2	611	U
1	S2	617	U
1	S2	619	A
1	S2	620	A
1	S2	623	A
1	S2	624	G
1	S2	635	A
1	S2	638	U
1	S2	639	U
1	S2	640	U
1	S2	641	G
1	S2	643	G
1	S2	645	C
1	S2	651	G
1	S2	653	C
1	S2	654	C
1	S2	655	G
1	S2	656	G
1	S2	677	G
1	S2	678	A
1	S2	680	U
1	S2	682	C
1	S2	684	A
1	S2	687	G
1	S2	693	U
1	S2	694	U
1	S2	696	C
1	S2	697	C
1	S2	698	U
1	S2	700	C
1	S2	702	G
1	S2	703	G
1	S2	704	C
1	S2	705	U
1	S2	706	A
1	S2	707	A
1	S2	708	C
1	S2	709	C
1	S2	710	U

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Mol	Chain	Res	Type
1	S2	711	U
1	S2	712	G
1	S2	714	G
1	S2	728	U
1	S2	729	G
1	S2	730	G
1	S2	732	G
1	S2	733	A
1	S2	736	C
1	S2	738	G
1	S2	739	G
1	S2	741	C
1	S2	742	U
1	S2	743	U
1	S2	744	U
1	S2	745	U
1	S2	753	A
1	S2	755	A
1	S2	756	A
1	S2	765	G
1	S2	766	U
1	S2	771	A
1	S2	774	A
1	S2	775	G
1	S2	778	G
1	S2	781	U
1	S2	782	U
1	S2	783	G
1	S2	787	G
1	S2	789	A
1	S2	794	U
1	S2	804	A
1	S2	807	A
1	S2	812	A
1	S2	813	U
1	S2	814	A
1	S2	815	G
1	S2	816	G
1	S2	818	C
1	S2	819	G
1	S2	820	U
1	S2	821	U

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Mol	Chain	Res	Type
1	S2	823	G
1	S2	832	U
1	S2	833	U
1	S2	836	U
1	S2	837	G
1	S2	839	U
1	S2	840	U
1	S2	841	U
1	S2	846	G
1	S2	851	U
1	S2	852	C
1	S2	855	A
1	S2	856	A
1	S2	857	U
1	S2	863	A
1	S2	865	A
1	S2	873	U
1	S2	876	G
1	S2	877	G
1	S2	886	U
1	S2	898	A
1	S2	899	G
1	S2	901	G
1	S2	902	G
1	S2	904	G
1	S2	912	U
1	S2	913	G
1	S2	929	A
1	S2	932	U
1	S2	933	A
1	S2	934	C
1	S2	935	U
1	S2	940	A
1	S2	945	U
1	S2	960	U
1	S2	964	U
1	S2	966	A
1	S2	970	A
1	S2	973	A
1	S2	977	A
1	S2	988	A
1	S2	989	U

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Mol	Chain	Res	Type
1	S2	992	A
1	S2	996	U
1	S2	998	A
1	S2	1001	A
1	S2	1004	U
1	S2	1024	U
1	S2	1026	A
1	S2	1028	C
1	S2	1029	U
1	S2	1032	G
1	S2	1039	A
1	S2	1040	G
1	S2	1052	U
1	S2	1053	G
1	S2	1057	U
1	S2	1058	U
1	S2	1059	U
1	S2	1060	U
1	S2	1061	A
1	S2	1062	A
1	S2	1063	U
1	S2	1074	G
1	S2	1080	U
1	S2	1081	A
1	S2	1082	C
1	S2	1092	A
1	S2	1096	C
1	S2	1099	U
1	S2	1100	G
1	S2	1109	G
1	S2	1111	G
1	S2	1113	A
1	S2	1138	A
1	S2	1156	C
1	S2	1158	C
1	S2	1160	A
1	S2	1164	G
1	S2	1167	G
1	S2	1170	G
1	S2	1183	A
1	S2	1185	U
1	S2	1186	U

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Mol	Chain	Res	Type
1	S2	1187	U
1	S2	1191	U
1	S2	1194	A
1	S2	1196	A
1	S2	1197	C
1	S2	1199	G
1	S2	1200	G
1	S2	1208	A
1	S2	1212	G
1	S2	1214	U
1	S2	1217	A
1	S2	1218	G
1	S2	1227	A
1	S2	1229	G
1	S2	1241	G
1	S2	1243	G
1	S2	1244	A
1	S2	1245	G
1	S2	1246	C
1	S2	1252	C
1	S2	1256	A
1	S2	1257	U
1	S2	1258	U
1	S2	1263	G
1	S2	1264	G
1	S2	1265	G
1	S2	1269	U
1	S2	1273	G
1	S2	1274	C
1	S2	1275	A
1	S2	1276	U
1	S2	1285	U
1	S2	1294	G
1	S2	1301	U
1	S2	1307	U
1	S2	1314	U
1	S2	1315	U
1	S2	1318	G
1	S2	1321	A
1	S2	1322	A
1	S2	1325	A
1	S2	1337	A

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Mol	Chain	Res	Type
1	S2	1341	A
1	S2	1344	A
1	S2	1345	A
1	S2	1346	A
1	S2	1348	A
1	S2	1349	G
1	S2	1354	G
1	S2	1360	A
1	S2	1361	U
1	S2	1363	U
1	S2	1367	G
1	S2	1370	U
1	S2	1371	A
1	S2	1372	U
1	S2	1373	C
1	S2	1381	U
1	S2	1382	A
1	S2	1383	G
1	S2	1385	G
1	S2	1390	U
1	S2	1398	U
1	S2	1399	C
1	S2	1400	A
1	S2	1402	G
1	S2	1414	U
1	S2	1415	U
1	S2	1421	A
1	S2	1427	A
1	S2	1431	C
1	S2	1432	U
1	S2	1433	G
1	S2	1446	A
1	S2	1447	C
1	S2	1448	G
1	S2	1457	C
1	S2	1458	G
1	S2	1459	C
1	S2	1460	A
1	S2	1469	A
1	S2	1472	C
1	S2	1473	U
1	S2	1479	A

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Mol	Chain	Res	Type
1	S2	1482	C
1	S2	1483	A
1	S2	1488	G
1	S2	1489	U
1	S2	1490	C
1	S2	1491	U
1	S2	1492	A
1	S2	1493	A
1	S2	1496	U
1	S2	1510	U
1	S2	1514	U
1	S2	1515	A
1	S2	1516	A
1	S2	1517	U
1	S2	1518	C
1	S2	1521	G
1	S2	1523	G
1	S2	1524	A
1	S2	1528	U
1	S2	1529	C
1	S2	1531	G
1	S2	1537	C
1	S2	1540	G
1	S2	1543	A
1	S2	1545	A
1	S2	1556	A
1	S2	1557	U
1	S2	1558	U
1	S2	1559	A
1	S2	1572	G
1	S2	1573	A
1	S2	1574	G
1	S2	1575	G
1	S2	1576	A
1	S2	1583	A
1	S2	1584	G
1	S2	1585	U
1	S2	1590	G
1	S2	1592	A
1	S2	1601	G
1	S2	1607	G
1	S2	1611	A

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Mol	Chain	Res	Type
1	S2	1614	A
1	S2	1616	G
1	S2	1619	C
1	S2	1622	G
1	S2	1634	C
1	S2	1637	C
1	S2	1657	U
1	S2	1658	G
1	S2	1660	A
1	S2	1673	G
1	S2	1676	U
1	S2	1682	U
1	S2	1688	U
1	S2	1689	A
1	S2	1693	A
1	S2	1700	C
1	S2	1701	A
1	S2	1702	A
1	S2	1703	C
1	S2	1709	C
1	S2	1711	C
1	S2	1715	G
1	S2	1717	G
1	S2	1736	G
1	S2	1740	A
1	S2	1755	A
1	S2	1757	G
1	S2	1760	G
1	S2	1762	A
1	S2	1766	A
1	S2	1767	G
1	S2	1769	U
1	S2	1770	U
1	S2	1780	G
1	S2	1782	A
1	S2	1783	C
1	S2	1788	G
1	S2	1792	G
1	S2	1793	G
1	S2	1794	A
1	S2	1796	C
1	S2	1799	U

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Mol	Chain	Res	Type
2	Sl	2	U
36	Sm	3	G
36	Sm	8	U
36	Sm	10	G
36	Sm	14	A
36	Sm	15	G
36	Sm	16	U
36	Sm	19	G
36	Sm	20	U
36	Sm	21	A
36	Sm	34	U
36	Sm	35	U
36	Sm	46	G
36	Sm	47	U
36	Sm	48	C
36	Sm	49	G
36	Sm	50	C
36	Sm	51	A
36	Sm	52	G
36	Sm	53	G
36	Sm	54	U
36	Sm	55	U
36	Sm	57	G
36	Sm	58	A
36	Sm	59	A
36	Sm	60	U
36	Sm	61	C
36	Sm	62	C
36	Sm	64	G
36	Sm	65	C
36	Sm	66	A
36	Sm	67	C
36	Sm	68	G
36	Sm	69	A
36	Sm	73	A
36	Sm	74	C
37	Sn	8	U
37	Sn	9	G
37	Sn	11	C
37	Sn	14	A
37	Sn	19	G
37	Sn	20	A

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Mol	Chain	Res	Type
37	Sn	21	A
37	Sn	25	C
37	Sn	27	C
37	Sn	36	U
37	Sn	45	U
37	Sn	46	G
37	Sn	47	U
37	Sn	48	C
37	Sn	49	C
37	Sn	54	A
37	Sn	57	G
37	Sn	59	A
37	Sn	61	C
37	Sn	63	G
37	Sn	64	A
37	Sn	66	C
37	Sn	76	A
40	LA	6	A
40	LA	11	A
40	LA	14	U
40	LA	21	G
40	LA	22	G
40	LA	26	A
40	LA	30	G
40	LA	40	A
40	LA	43	A
40	LA	44	U
40	LA	48	A
40	LA	49	A
40	LA	51	A
40	LA	59	G
40	LA	60	A
40	LA	65	A
40	LA	66	A
40	LA	73	C
40	LA	74	G
40	LA	76	G
40	LA	85	A
40	LA	89	A
40	LA	92	G
40	LA	109	A
40	LA	110	G

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Mol	Chain	Res	Type
40	LA	111	C
40	LA	113	C
40	LA	120	G
40	LA	121	A
40	LA	122	A
40	LA	133	U
40	LA	136	G
40	LA	150	A
40	LA	156	G
40	LA	157	A
40	LA	166	C
40	LA	173	G
40	LA	187	A
40	LA	190	U
40	LA	191	U
40	LA	200	C
40	LA	206	G
40	LA	210	U
40	LA	211	A
40	LA	213	A
40	LA	218	G
40	LA	219	A
40	LA	221	A
40	LA	231	G
40	LA	236	G
40	LA	239	G
40	LA	240	U
40	LA	243	G
40	LA	249	U
40	LA	252	U
40	LA	258	G
40	LA	263	C
40	LA	269	G
40	LA	282	G
40	LA	283	G
40	LA	286	U
40	LA	295	A
40	LA	298	U
40	LA	315	C
40	LA	323	A
40	LA	329	U
40	LA	330	G

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Mol	Chain	Res	Type
40	LA	334	A
40	LA	338	A
40	LA	339	C
40	LA	346	C
40	LA	350	C
40	LA	351	A
40	LA	376	G
40	LA	385	A
40	LA	390	G
40	LA	395	A
40	LA	397	A
40	LA	399	A
40	LA	401	U
40	LA	402	A
40	LA	403	C
40	LA	421	G
40	LA	422	A
40	LA	438	A
40	LA	440	A
40	LA	441	U
40	LA	442	G
40	LA	443	G
40	LA	445	G
40	LA	446	U
40	LA	447	U
40	LA	448	U
40	LA	449	U
40	LA	450	G
40	LA	487	U
40	LA	488	U
40	LA	489	U
40	LA	490	C
40	LA	491	A
40	LA	492	C
40	LA	494	G
40	LA	498	A
40	LA	510	G
40	LA	515	C
40	LA	517	G
40	LA	520	U
40	LA	521	A
40	LA	535	G

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Mol	Chain	Res	Type
40	LA	543	C
40	LA	544	C
40	LA	545	U
40	LA	546	C
40	LA	547	G
40	LA	552	G
40	LA	555	U
40	LA	557	A
40	LA	559	A
40	LA	568	G
40	LA	578	A
40	LA	579	G
40	LA	597	G
40	LA	600	G
40	LA	603	A
40	LA	604	G
40	LA	609	G
40	LA	610	G
40	LA	611	A
40	LA	612	U
40	LA	619	A
40	LA	620	U
40	LA	621	A
40	LA	625	G
40	LA	637	C
40	LA	638	C
40	LA	642	U
40	LA	649	A
40	LA	650	C
40	LA	660	A
40	LA	667	C
40	LA	677	A
40	LA	681	U
40	LA	691	A
40	LA	699	A
40	LA	705	A
40	LA	712	G
40	LA	716	A
40	LA	720	A
40	LA	726	G
40	LA	737	G
40	LA	742	G

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Mol	Chain	Res	Type
40	LA	758	C
40	LA	763	G
40	LA	764	U
40	LA	765	C
40	LA	766	U
40	LA	767	U
40	LA	771	A
40	LA	774	G
40	LA	776	U
40	LA	777	U
40	LA	780	A
40	LA	781	G
40	LA	785	G
40	LA	786	A
40	LA	806	A
40	LA	808	A
40	LA	817	A
40	LA	830	A
40	LA	832	G
40	LA	848	A
40	LA	849	C
40	LA	850	U
40	LA	851	C
40	LA	861	C
40	LA	865	U
40	LA	868	C
40	LA	871	U
40	LA	874	U
40	LA	879	U
40	LA	894	G
40	LA	895	A
40	LA	896	A
40	LA	899	U
40	LA	906	A
40	LA	907	G
40	LA	908	G
40	LA	914	A
40	LA	916	G
40	LA	917	A
40	LA	921	A
40	LA	923	C
40	LA	932	U

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Mol	Chain	Res	Type
40	LA	934	G
40	LA	937	G
40	LA	944	C
40	LA	959	C
40	LA	960	U
40	LA	971	G
40	LA	974	G
40	LA	981	U
40	LA	982	C
40	LA	991	G
40	LA	1002	A
40	LA	1012	G
40	LA	1015	U
40	LA	1018	G
40	LA	1020	G
40	LA	1021	G
40	LA	1024	G
40	LA	1026	A
40	LA	1028	U
40	LA	1029	G
40	LA	1040	A
40	LA	1041	U
40	LA	1045	C
40	LA	1047	A
40	LA	1049	C
40	LA	1064	A
40	LA	1065	A
40	LA	1072	G
40	LA	1081	U
40	LA	1093	A
40	LA	1094	U
40	LA	1095	U
40	LA	1096	U
40	LA	1097	G
40	LA	1098	A
40	LA	1103	A
40	LA	1104	G
40	LA	1117	G
40	LA	1118	C
40	LA	1128	U
40	LA	1131	G
40	LA	1144	U

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Mol	Chain	Res	Type
40	LA	1145	G
40	LA	1148	G
40	LA	1153	A
40	LA	1158	A
40	LA	1159	A
40	LA	1177	G
40	LA	1178	G
40	LA	1180	A
40	LA	1181	U
40	LA	1182	A
40	LA	1190	A
40	LA	1192	C
40	LA	1193	A
40	LA	1196	C
40	LA	1197	A
40	LA	1201	C
40	LA	1202	A
40	LA	1206	G
40	LA	1208	U
40	LA	1217	A
40	LA	1218	U
40	LA	1222	G
40	LA	1223	A
40	LA	1227	C
40	LA	1229	G
40	LA	1234	G
40	LA	1236	G
40	LA	1237	G
40	LA	1238	C
40	LA	1239	C
40	LA	1240	A
40	LA	1241	U
40	LA	1242	G
40	LA	1243	G
40	LA	1244	A
40	LA	1245	A
40	LA	1246	G
40	LA	1248	C
40	LA	1251	A
40	LA	1253	U
40	LA	1258	U
40	LA	1262	G

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Mol	Chain	Res	Type
40	LA	1263	A
40	LA	1264	G
40	LA	1266	G
40	LA	1267	U
40	LA	1269	U
40	LA	1270	A
40	LA	1271	A
40	LA	1272	C
40	LA	1278	A
40	LA	1279	C
40	LA	1280	C
40	LA	1282	G
40	LA	1285	G
40	LA	1286	A
40	LA	1287	A
40	LA	1295	G
40	LA	1307	G
40	LA	1308	A
40	LA	1309	U
40	LA	1313	G
40	LA	1316	C
40	LA	1318	A
40	LA	1325	U
40	LA	1330	A
40	LA	1345	G
40	LA	1348	U
40	LA	1349	G
40	LA	1351	U
40	LA	1352	A
40	LA	1354	G
40	LA	1355	A
40	LA	1356	U
40	LA	1357	G
40	LA	1386	A
40	LA	1392	G
40	LA	1399	A
40	LA	1400	G
40	LA	1418	A
40	LA	1419	A
40	LA	1421	G
40	LA	1429	G
40	LA	1430	U

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Mol	Chain	Res	Type
40	LA	1431	G
40	LA	1434	G
40	LA	1437	C
40	LA	1442	U
40	LA	1443	G
40	LA	1446	A
40	LA	1450	G
40	LA	1455	U
40	LA	1481	A
40	LA	1482	A
40	LA	1483	G
40	LA	1484	U
40	LA	1487	G
40	LA	1488	G
40	LA	1503	A
40	LA	1508	C
40	LA	1511	U
40	LA	1523	U
40	LA	1528	G
40	LA	1533	U
40	LA	1536	G
40	LA	1542	G
40	LA	1549	U
40	LA	1555	U
40	LA	1556	C
40	LA	1557	A
40	LA	1559	A
40	LA	1560	G
40	LA	1562	C
40	LA	1563	C
40	LA	1565	G
40	LA	1566	A
40	LA	1567	U
40	LA	1568	U
40	LA	1569	U
40	LA	1572	U
40	LA	1573	G
40	LA	1574	C
40	LA	1575	A
40	LA	1576	G
40	LA	1580	A
40	LA	1581	C

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Mol	Chain	Res	Type
40	LA	1582	C
40	LA	1583	A
40	LA	1587	A
40	LA	1588	A
40	LA	1589	A
40	LA	1590	G
40	LA	1602	A
40	LA	1605	A
40	LA	1621	A
40	LA	1629	U
40	LA	1632	A
40	LA	1639	C
40	LA	1642	A
40	LA	1643	A
40	LA	1645	U
40	LA	1658	G
40	LA	1677	G
40	LA	1683	A
40	LA	1687	U
40	LA	1688	U
40	LA	1696	A
40	LA	1704	A
40	LA	1705	U
40	LA	1715	A
40	LA	1716	U
40	LA	1717	U
40	LA	1722	U
40	LA	1724	U
40	LA	1725	C
40	LA	1750	A
40	LA	1751	G
40	LA	1756	C
40	LA	1760	A
40	LA	1765	U
40	LA	1766	G
40	LA	1770	G
40	LA	1775	G
40	LA	1780	G
40	LA	1788	C
40	LA	1796	G
40	LA	1797	A
40	LA	1814	A

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Mol	Chain	Res	Type
40	LA	1816	A
40	LA	1817	G
40	LA	1819	U
40	LA	1820	U
40	LA	1821	U
40	LA	1822	C
40	LA	1839	A
40	LA	1840	U
40	LA	1841	A
40	LA	1842	A
40	LA	1846	C
40	LA	1849	C
40	LA	1850	A
40	LA	1866	C
40	LA	1867	A
40	LA	1874	A
40	LA	1880	U
40	LA	1881	A
40	LA	1893	A
40	LA	1897	G
40	LA	1906	G
40	LA	1908	A
40	LA	1930	A
40	LA	1935	G
40	LA	1943	C
40	LA	1951	C
40	LA	1952	G
40	LA	1953	G
40	LA	1954	G
40	LA	2101	C
40	LA	2102	U
40	LA	2111	G
40	LA	2112	U
40	LA	2113	A
40	LA	2121	G
40	LA	2122	G
40	LA	2131	A
40	LA	2139	A
40	LA	2149	A
40	LA	2158	A
40	LA	2169	G
40	LA	2170	U

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Mol	Chain	Res	Type
40	LA	2187	G
40	LA	2188	A
40	LA	2201	G
40	LA	2205	U
40	LA	2206	G
40	LA	2207	A
40	LA	2209	U
40	LA	2223	A
40	LA	2232	A
40	LA	2244	A
40	LA	2249	G
40	LA	2250	G
40	LA	2252	A
40	LA	2256	A
40	LA	2262	A
40	LA	2272	G
40	LA	2273	G
40	LA	2274	U
40	LA	2279	A
40	LA	2280	A
40	LA	2281	A
40	LA	2282	U
40	LA	2284	C
40	LA	2285	C
40	LA	2288	G
40	LA	2299	A
40	LA	2306	C
40	LA	2307	G
40	LA	2308	C
40	LA	2309	A
40	LA	2310	U
40	LA	2313	A
40	LA	2314	U
40	LA	2315	G
40	LA	2335	G
40	LA	2336	U
40	LA	2347	U
40	LA	2364	G
40	LA	2372	A
40	LA	2373	A
40	LA	2374	C
40	LA	2375	G

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Mol	Chain	Res	Type
40	LA	2385	G
40	LA	2388	U
40	LA	2393	G
40	LA	2394	G
40	LA	2397	A
40	LA	2402	A
40	LA	2403	G
40	LA	2404	A
40	LA	2411	U
40	LA	2412	G
40	LA	2419	A
40	LA	2422	C
40	LA	2434	U
40	LA	2435	G
40	LA	2437	G
40	LA	2438	A
40	LA	2439	A
40	LA	2440	G
40	LA	2446	U
40	LA	2451	G
40	LA	2452	G
40	LA	2493	U
40	LA	2496	C
40	LA	2498	U
40	LA	2501	U
40	LA	2502	A
40	LA	2503	G
40	LA	2507	C
40	LA	2514	U
40	LA	2515	A
40	LA	2522	G
40	LA	2523	A
40	LA	2524	A
40	LA	2525	G
40	LA	2526	C
40	LA	2531	C
40	LA	2532	U
40	LA	2537	U
40	LA	2538	U
40	LA	2539	C
40	LA	2540	A
40	LA	2541	U

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Mol	Chain	Res	Type
40	LA	2542	U
40	LA	2543	U
40	LA	2546	C
40	LA	2549	G
40	LA	2552	C
40	LA	2554	A
40	LA	2561	A
40	LA	2569	A
40	LA	2570	U
40	LA	2571	U
40	LA	2572	C
40	LA	2573	G
40	LA	2576	G
40	LA	2585	G
40	LA	2589	G
40	LA	2593	A
40	LA	2594	C
40	LA	2595	A
40	LA	2606	G
40	LA	2607	G
40	LA	2614	G
40	LA	2626	A
40	LA	2629	U
40	LA	2636	A
40	LA	2648	G
40	LA	2652	U
40	LA	2656	A
40	LA	2672	G
40	LA	2674	A
40	LA	2677	G
40	LA	2689	A
40	LA	2691	A
40	LA	2694	A
40	LA	2696	A
40	LA	2703	A
40	LA	2704	A
40	LA	2714	G
40	LA	2719	U
40	LA	2728	G
40	LA	2748	A
40	LA	2749	G
40	LA	2752	U

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Mol	Chain	Res	Type
40	LA	2753	G
40	LA	2755	C
40	LA	2777	G
40	LA	2778	G
40	LA	2796	G
40	LA	2800	G
40	LA	2801	A
40	LA	2802	A
40	LA	2803	A
40	LA	2804	A
40	LA	2805	G
40	LA	2810	C
40	LA	2817	A
40	LA	2818	U
40	LA	2821	C
40	LA	2842	U
40	LA	2844	C
40	LA	2845	A
40	LA	2847	A
40	LA	2849	C
40	LA	2856	G
40	LA	2861	U
40	LA	2867	C
40	LA	2871	G
40	LA	2872	A
40	LA	2873	U
40	LA	2875	U
40	LA	2876	C
40	LA	2887	A
40	LA	2894	C
40	LA	2899	C
40	LA	2910	A
40	LA	2916	U
40	LA	2918	G
40	LA	2923	U
40	LA	2928	C
40	LA	2933	A
40	LA	2935	U
40	LA	2936	A
40	LA	2941	A
40	LA	2942	C
40	LA	2947	G

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Mol	Chain	Res	Type
40	LA	2954	U
40	LA	2955	U
40	LA	2957	G
40	LA	2971	A
40	LA	2983	C
40	LA	2990	G
40	LA	2996	U
40	LA	2997	G
40	LA	3003	G
40	LA	3012	A
40	LA	3030	G
40	LA	3056	U
40	LA	3058	U
40	LA	3059	G
40	LA	3078	U
40	LA	3079	U
40	LA	3080	G
40	LA	3086	A
40	LA	3092	C
40	LA	3101	G
40	LA	3104	U
40	LA	3115	C
40	LA	3116	G
40	LA	3118	C
40	LA	3119	U
40	LA	3122	A
40	LA	3129	A
40	LA	3130	A
40	LA	3131	U
40	LA	3142	A
40	LA	3143	C
40	LA	3151	U
40	LA	3154	C
40	LA	3155	U
40	LA	3156	U
40	LA	3157	U
40	LA	3158	G
40	LA	3165	A
40	LA	3170	A
40	LA	3172	A
40	LA	3173	G
40	LA	3174	A

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Mol	Chain	Res	Type
40	LA	3175	U
40	LA	3176	G
40	LA	3180	A
40	LA	3181	C
40	LA	3187	A
40	LA	3196	U
40	LA	3199	G
40	LA	3207	U
40	LA	3209	A
40	LA	3210	A
40	LA	3216	G
40	LA	3217	C
40	LA	3218	A
40	LA	3219	G
40	LA	3222	U
40	LA	3229	G
40	LA	3242	G
40	LA	3243	A
40	LA	3244	A
40	LA	3245	A
40	LA	3247	G
40	LA	3259	U
40	LA	3260	G
40	LA	3263	G
40	LA	3270	U
40	LA	3273	A
40	LA	3276	G
40	LA	3277	U
40	LA	3281	U
40	LA	3286	G
40	LA	3287	U
40	LA	3288	G
40	LA	3289	G
40	LA	3294	A
40	LA	3295	A
40	LA	3304	U
40	LA	3313	U
40	LA	3316	A
40	LA	3318	G
40	LA	3319	U
40	LA	3320	A
40	LA	3334	U

*Continued on next page...*

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Mol	Chain	Res	Type
40	LA	3341	U
40	LA	3345	G
40	LA	3346	U
40	LA	3347	A
40	LA	3351	U
40	LA	3352	U
40	LA	3353	G
40	LA	3354	U
40	LA	3355	U
40	LA	3356	G
40	LA	3368	U
40	LA	3369	G
40	LA	3378	C
40	LA	3381	U
40	LA	3382	U
40	LA	3386	G
40	LA	3389	U
40	LA	3390	G
40	LA	3396	U
41	LB	7	G
41	LB	10	C
41	LB	17	A
41	LB	22	A
41	LB	35	C
41	LB	52	G
41	LB	53	U
41	LB	54	U
41	LB	65	G
41	LB	74	C
41	LB	76	A
41	LB	99	G
41	LB	102	A
41	LB	112	G
41	LB	121	U
42	LC	16	G
42	LC	25	G
42	LC	34	U
42	LC	35	C
42	LC	38	U
42	LC	59	A
42	LC	62	C
42	LC	63	G

*Continued on next page...*

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Mol	Chain	Res	Type
42	LC	80	A
42	LC	81	U
42	LC	82	U
42	LC	83	C
42	LC	84	C
42	LC	85	G
42	LC	86	U
42	LC	87	G
42	LC	90	U
42	LC	95	G
42	LC	97	A
42	LC	99	C
42	LC	104	A
42	LC	106	C
42	LC	111	A
42	LC	112	U
42	LC	113	U
42	LC	125	U
42	LC	126	A
42	LC	138	A
42	LC	148	G
42	LC	152	G
42	LC	157	U
42	LC	158	U

All (98) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	68	A
1	S2	77	U
1	S2	139	C
1	S2	141	U
1	S2	215	A
1	S2	224	C
1	S2	237	C
1	S2	278	U
1	S2	313	U
1	S2	322	G
1	S2	352	A
1	S2	387	A
1	S2	400	A
1	S2	447	U

*Continued on next page...*

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Mol	Chain	Res	Type
1	S2	511	A
1	S2	518	A
1	S2	539	G
1	S2	541	A
1	S2	555	A
1	S2	609	U
1	S2	639	U
1	S2	640	U
1	S2	705	U
1	S2	711	U
1	S2	740	A
1	S2	755	A
1	S2	803	A
1	S2	819	G
1	S2	912	U
1	S2	928	U
1	S2	1023	A
1	S2	1207	C
1	S2	1226	A
1	S2	1245	G
1	S2	1251	U
1	S2	1256	A
1	S2	1273	G
1	S2	1274	C
1	S2	1314	U
1	S2	1344	A
1	S2	1348	A
1	S2	1382	A
1	S2	1399	C
1	S2	1430	U
1	S2	1471	A
1	S2	1556	A
1	S2	1557	U
1	S2	1573	A
1	S2	1584	G
1	S2	1633	A
1	S2	1636	C
1	S2	1700	C
40	LA	13	A
40	LA	282	G
40	LA	439	C
40	LA	637	C

*Continued on next page...*

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Mol	Chain	Res	Type
40	LA	763	G
40	LA	849	C
40	LA	873	C
40	LA	896	A
40	LA	916	G
40	LA	993	G
40	LA	1064	A
40	LA	1097	G
40	LA	1271	A
40	LA	1307	G
40	LA	1355	A
40	LA	1562	C
40	LA	1572	U
40	LA	1582	C
40	LA	1716	U
40	LA	1815	U
40	LA	1820	U
40	LA	2112	U
40	LA	2231	C
40	LA	2445	A
40	LA	2500	A
40	LA	2501	U
40	LA	2502	A
40	LA	2513	U
40	LA	2514	U
40	LA	2525	G
40	LA	2537	U
40	LA	2538	U
40	LA	2541	U
40	LA	3055	U
40	LA	3078	U
40	LA	3121	U
40	LA	3218	A
40	LA	3228	C
40	LA	3269	U
40	LA	3275	U
40	LA	3319	U
40	LA	3350	C
41	LB	52	G
42	LC	82	U
42	LC	85	G
42	LC	125	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
84	5CT	Ls	51	84,40	13,14,15	2.31	1 (7%)	9,15,17	2.26	4 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	5CT	Ls	51	84,40	1/1/2/4	5/13/14/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Ls	51	5CT	O1-C2	-8.19	1.18	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	Ls	51	5CT	O1-C2-C3	3.62	119.57	109.21
84	Ls	51	5CT	O1-C2-C1	3.37	120.84	109.32
84	Ls	51	5CT	C3-C2-C1	3.26	119.58	112.16
84	Ls	51	5CT	C1-NZ-CE	-2.69	107.41	113.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
84	Ls	51	5CT	C2

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	Ls	51	5CT	C2-C1-NZ-CE
84	Ls	51	5CT	NZ-C1-C2-C3
84	Ls	51	5CT	O1-C2-C3-C4
84	Ls	51	5CT	C2-C3-C4-N1
84	Ls	51	5CT	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
86	A	13

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1104:ALA	C	1124:GLY	N	40.36
1	A	997:ALA	C	1019:ALA	N	35.44
1	A	1917:ALA	C	2000:ALA	N	14.67
1	A	1044:ALA	C	1055:ALA	N	12.76
1	A	1074:ALA	C	1084:ALA	N	11.98
1	A	2117:ALA	C	2200:ALA	N	11.35
1	A	2317:ALA	C	2320:ALA	N	6.51
1	A	1438:LEU	C	1441:ALA	N	5.15
1	A	1722:ALA	C	1800:ALA	N	4.52

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	987:ALA	C	988:ALA	N	3.81
1	A	1241:THR	C	1242:GLY	N	3.62
1	A	1486:ALA	C	1487:ALA	N	3.09
1	A	1221:ALA	C	1222:VAL	N	2.08



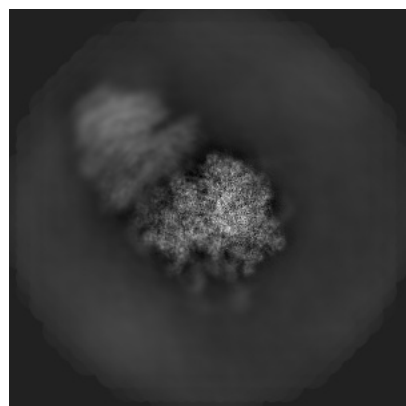
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12534. These allow visual inspection of the internal detail of the map and identification of artifacts.

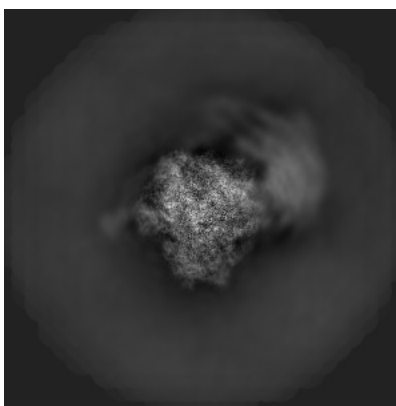
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

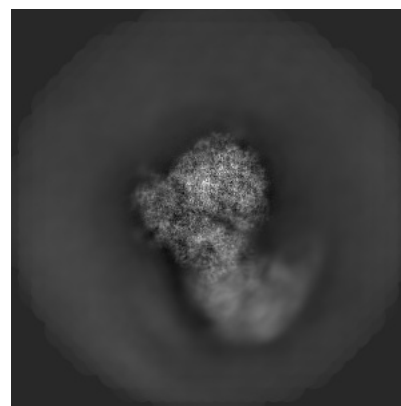
#### 6.1.1 Primary map



X

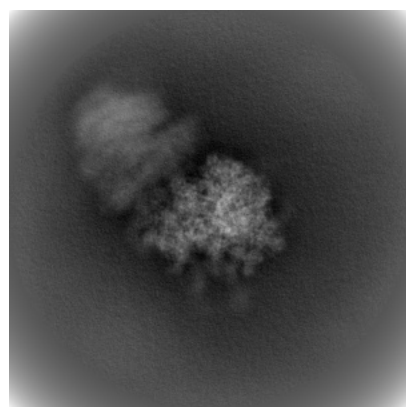


Y

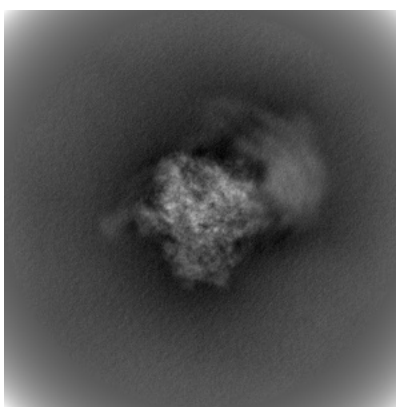


Z

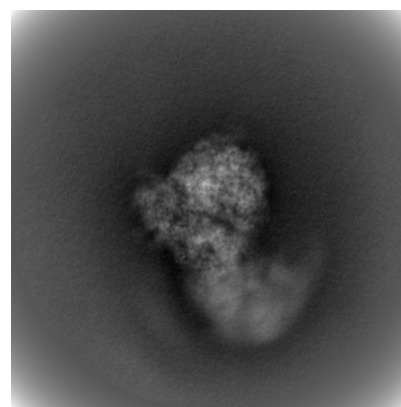
#### 6.1.2 Raw map



X



Y

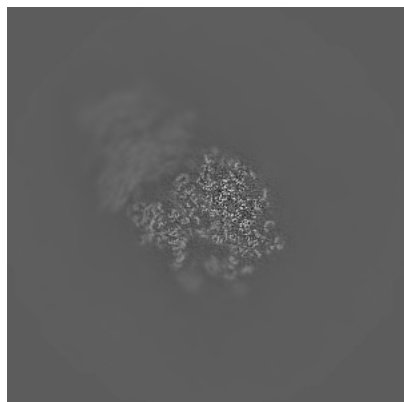


Z

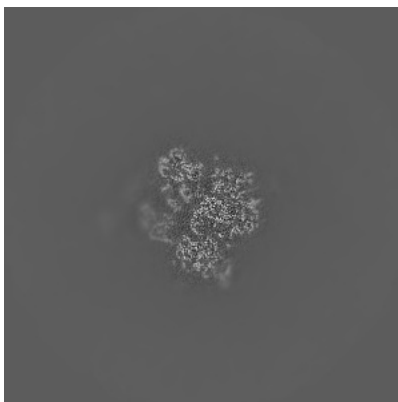
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

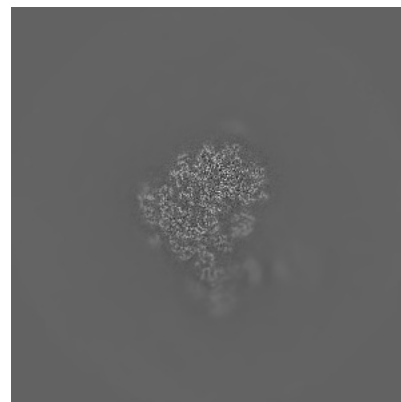
### 6.2.1 Primary map



X Index: 350

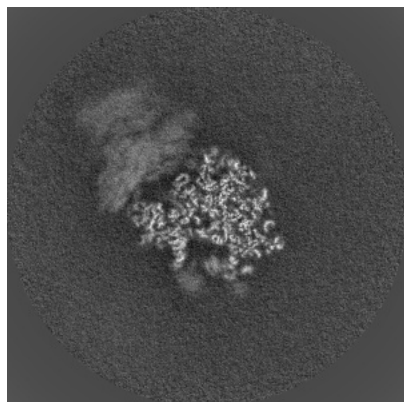


Y Index: 350

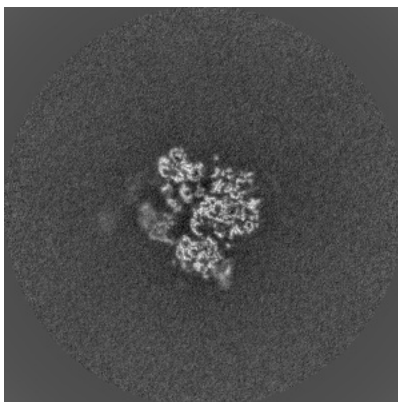


Z Index: 350

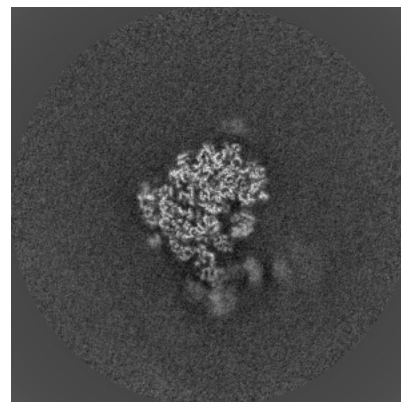
### 6.2.2 Raw map



X Index: 350



Y Index: 350

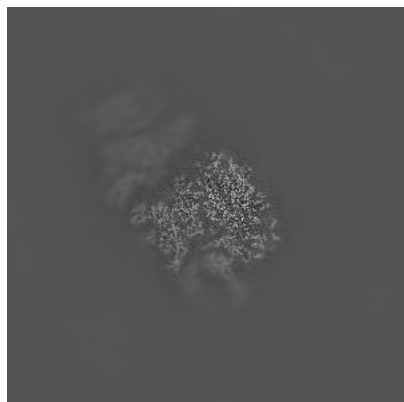


Z Index: 350

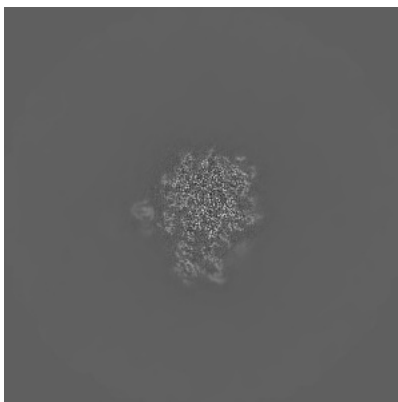
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 338

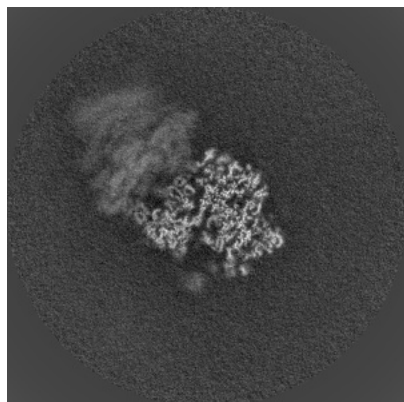


Y Index: 381

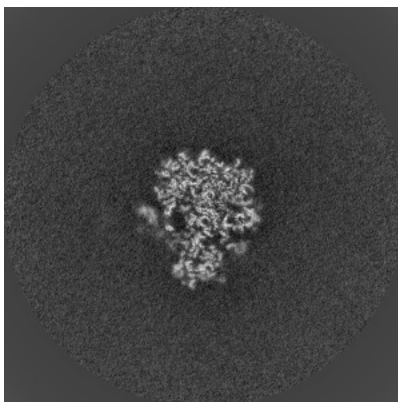


Z Index: 356

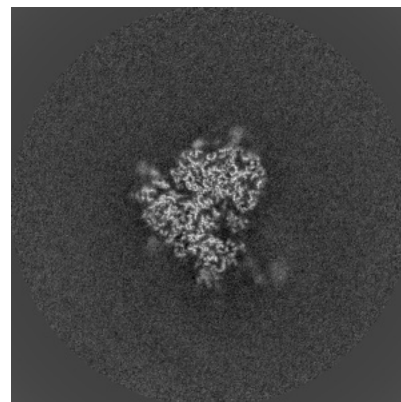
### 6.3.2 Raw map



X Index: 360



Y Index: 369

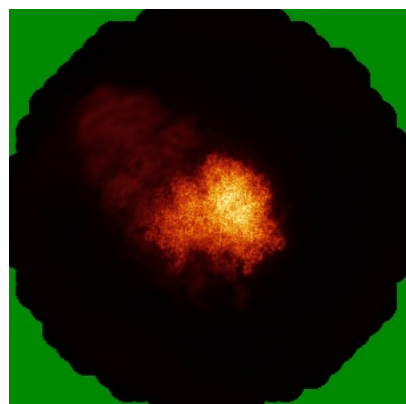


Z Index: 334

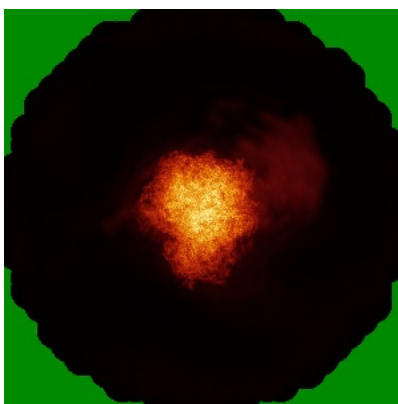
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

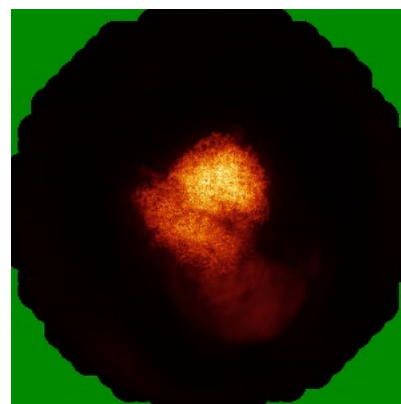
### 6.4.1 Primary map



X

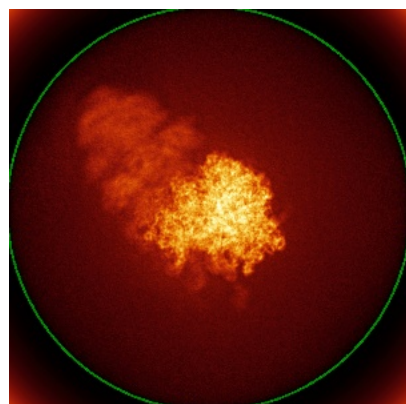


Y

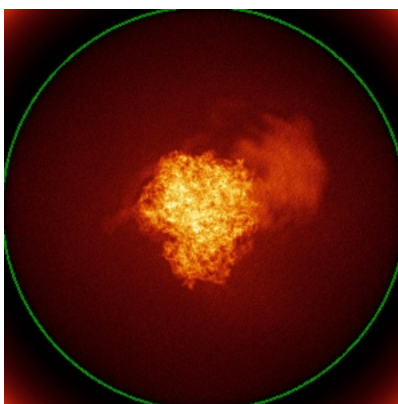


Z

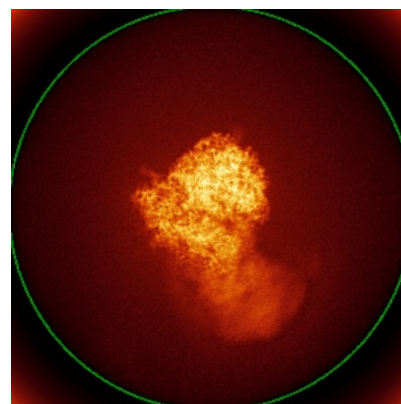
### 6.4.2 Raw map



X



Y

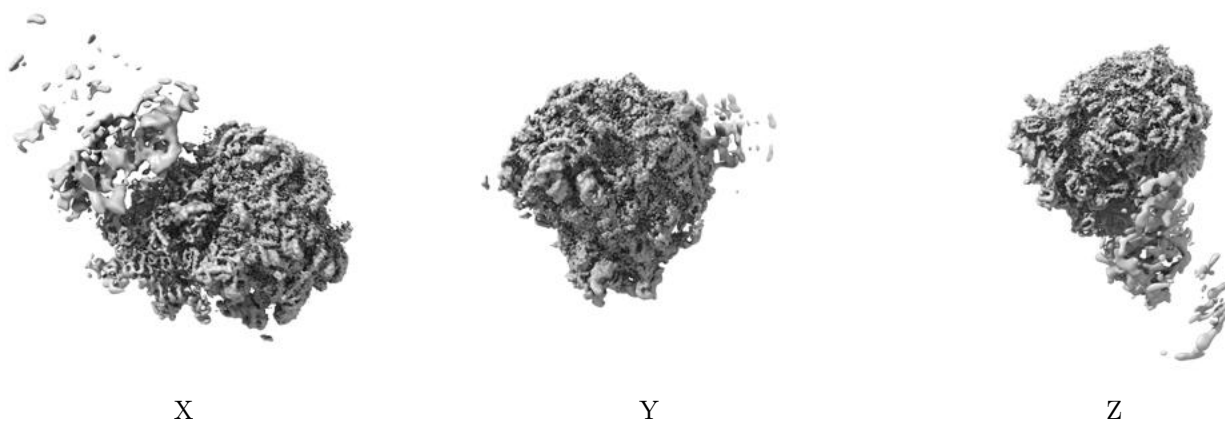


Z

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

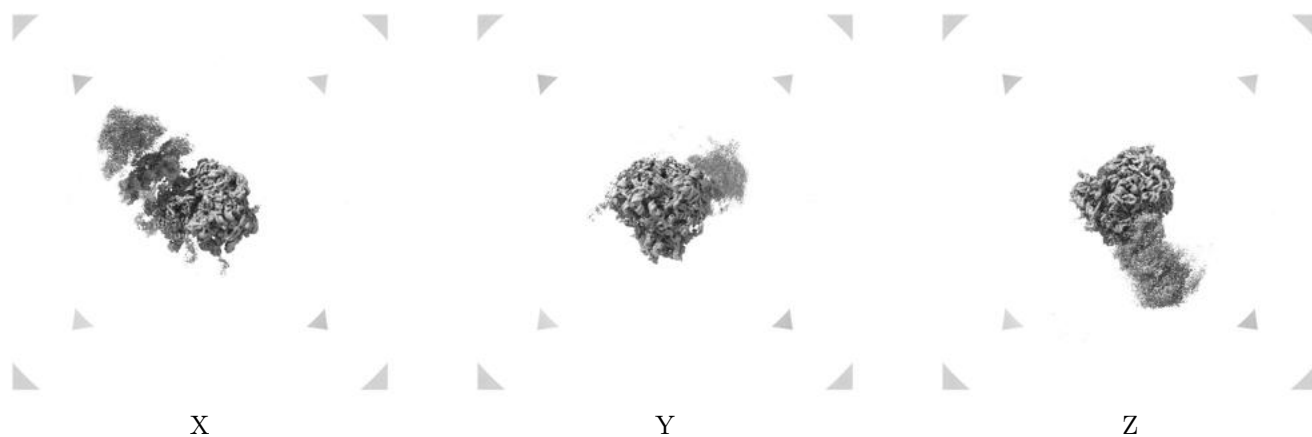
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

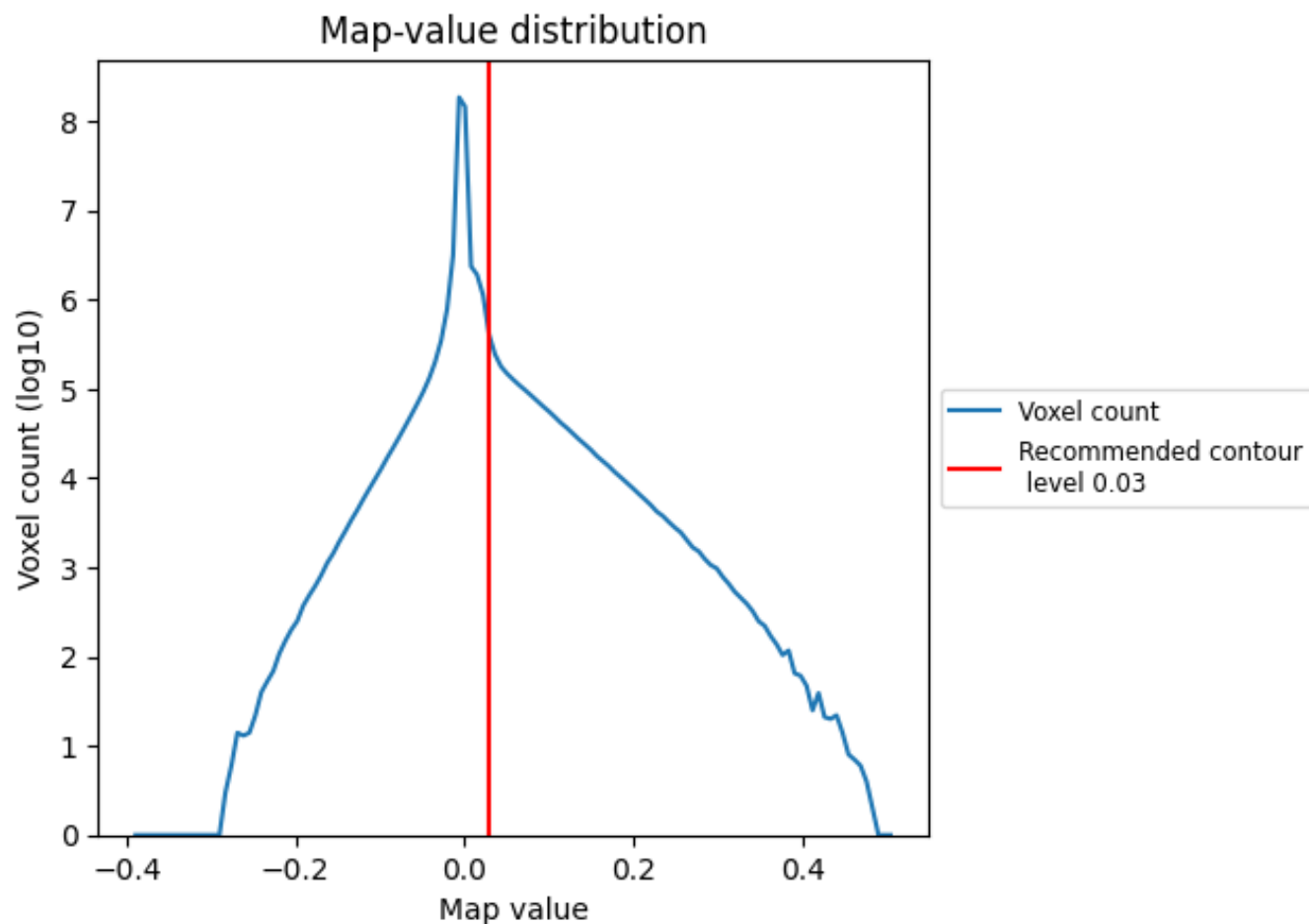
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

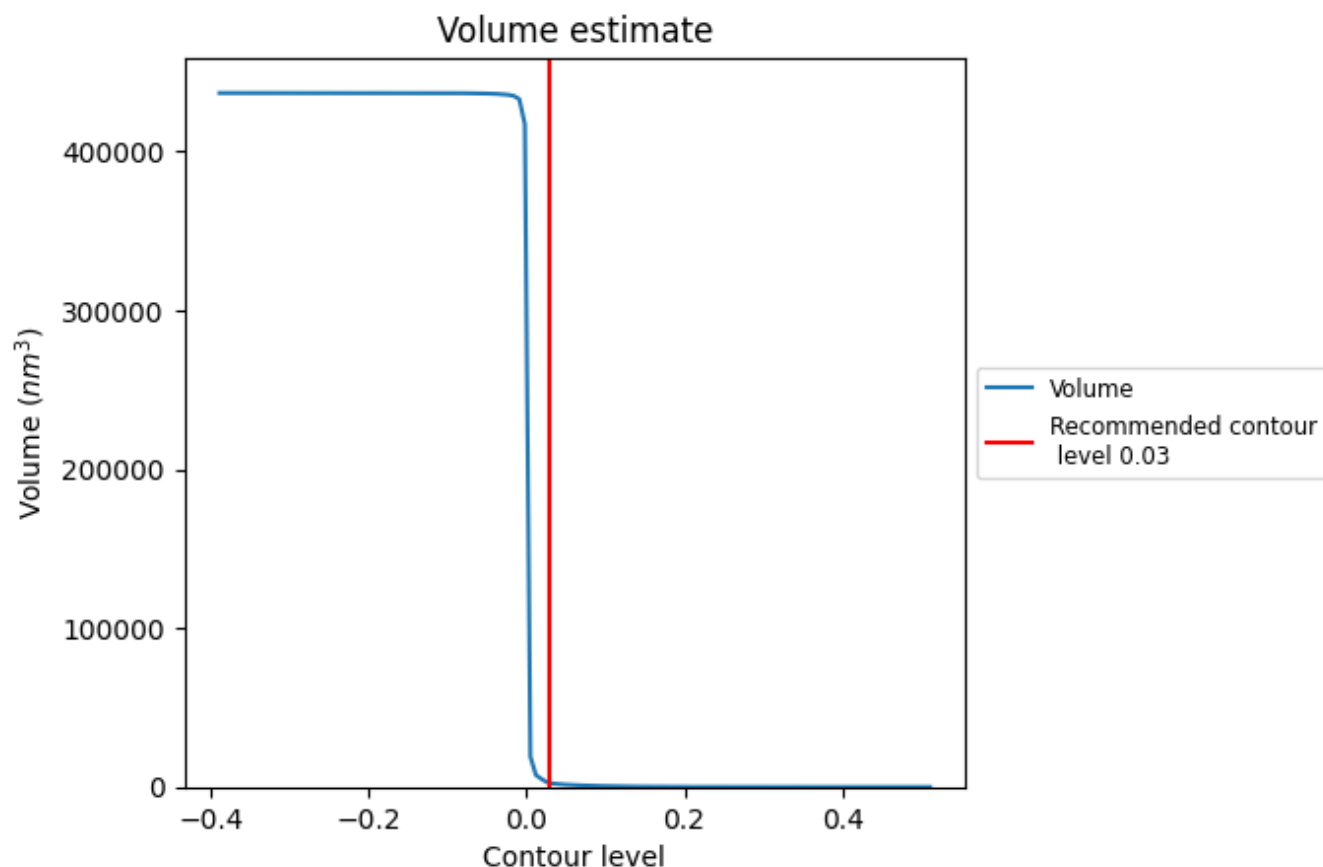
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

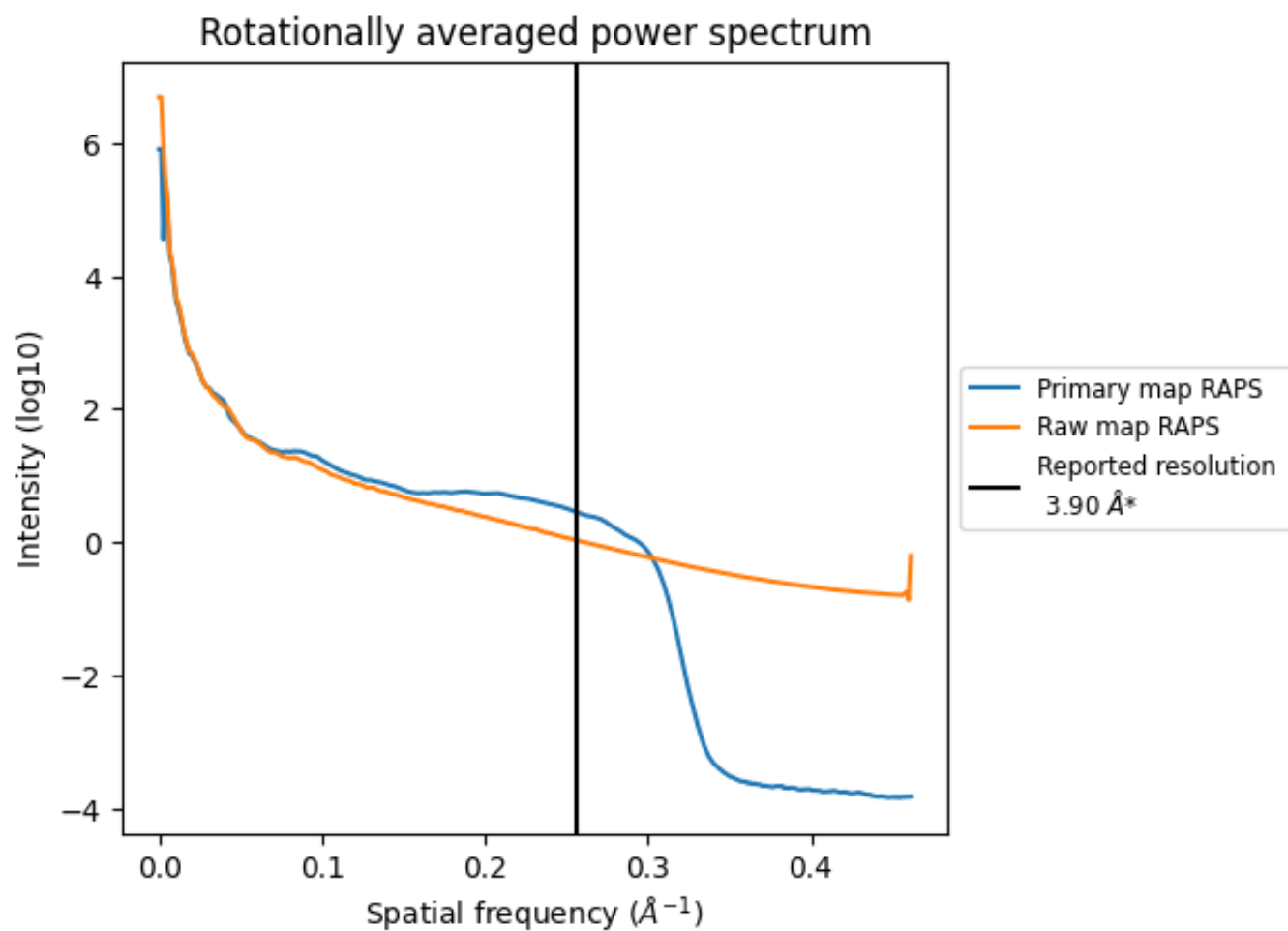


The volume at the recommended contour level is 2499  $\text{nm}^3$ ; this corresponds to an approximate mass of 2257 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ



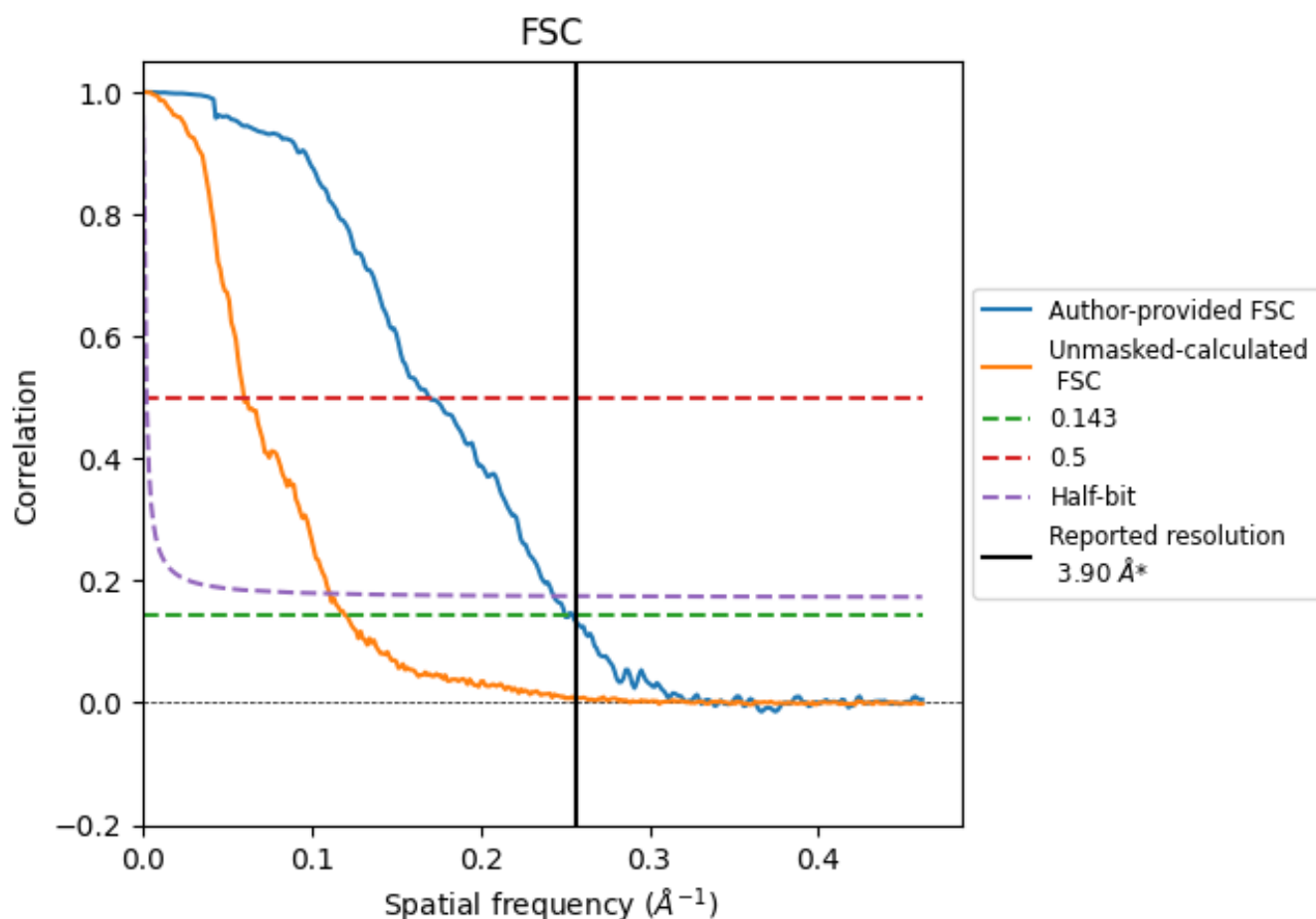
\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

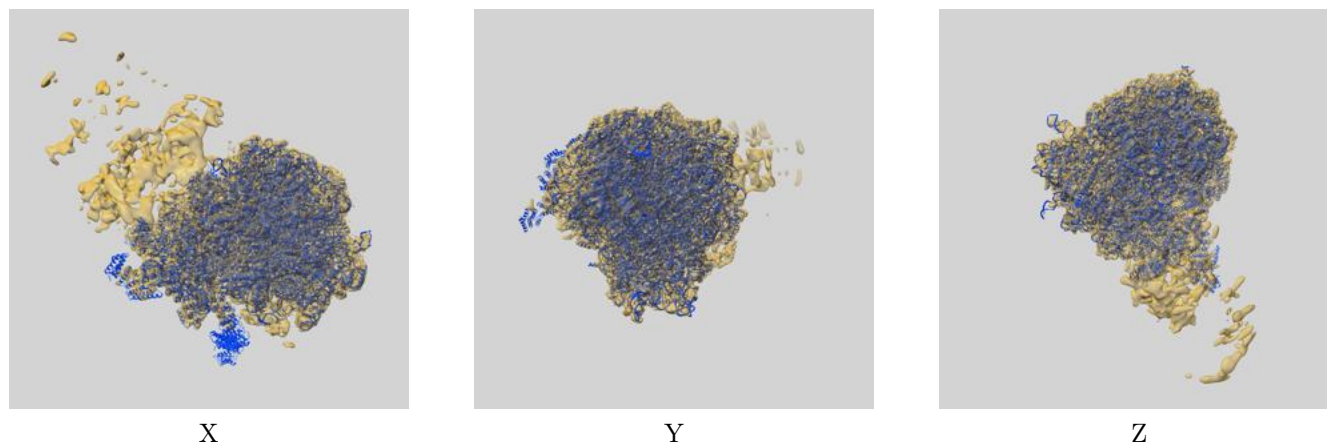
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	4.00	5.90	4.11
Unmasked-calculated*	8.33	16.61	9.03

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.33 differs from the reported value 3.9 by more than 10 %

## 9 Map-model fit [i](#)

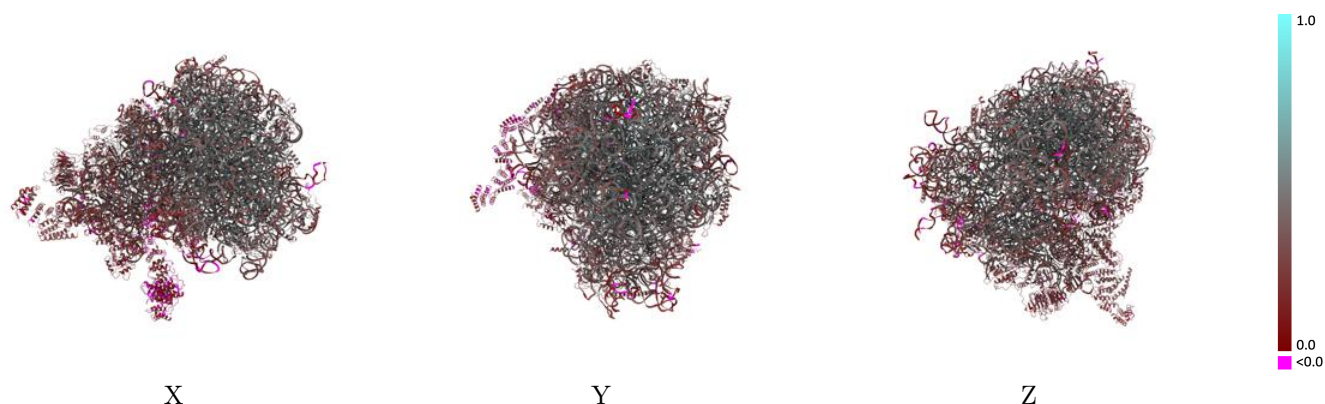
This section contains information regarding the fit between EMDB map EMD-12534 and PDB model 7NRC. Per-residue inclusion information can be found in section 3 on page 20.

### 9.1 Map-model overlay [i](#)



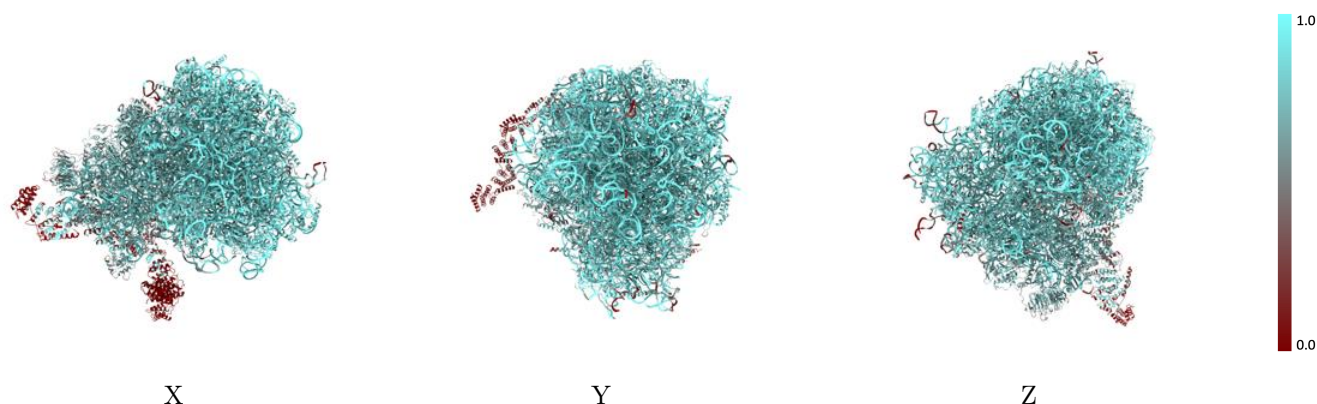
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



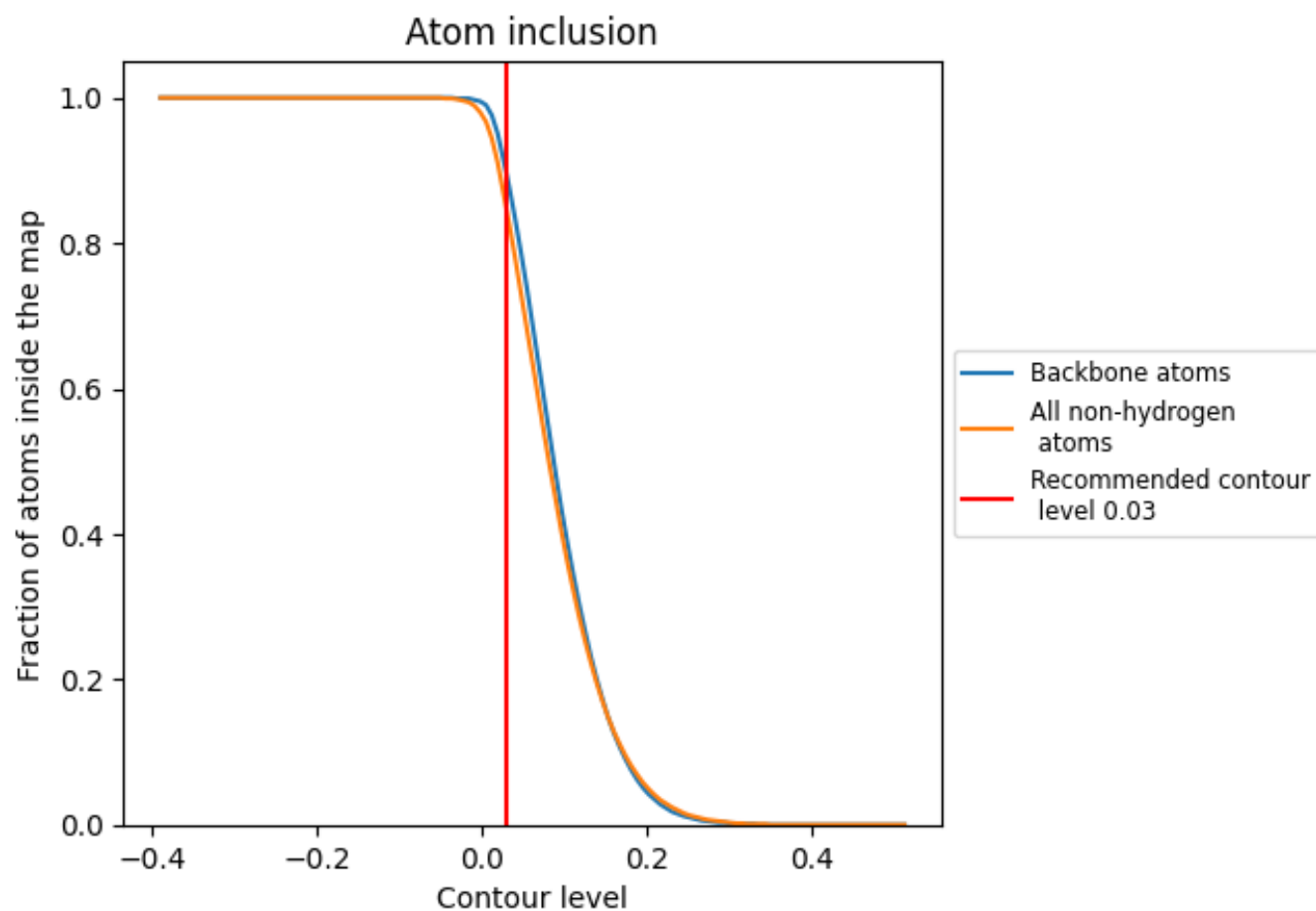
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.3780
A	 0.2820	 0.1550
LA	 0.9450	 0.4340
LB	 0.9490	 0.3610
LC	 0.9520	 0.4520
LD	 0.8640	 0.4660
LE	 0.8640	 0.4320
LF	 0.8480	 0.4070
LG	 0.7670	 0.2890
LH	 0.8260	 0.3730
LI	 0.8670	 0.4010
LJ	 0.8090	 0.3590
LK	 0.8110	 0.3720
LL	 0.7860	 0.3500
LM	 0.6150	 0.1650
LN	 0.8410	 0.3960
LO	 0.8610	 0.3760
LP	 0.8800	 0.4560
LQ	 0.8740	 0.4510
LR	 0.8630	 0.4320
LS	 0.8550	 0.4130
LT	 0.7830	 0.3720
LU	 0.8390	 0.4170
LV	 0.8430	 0.4050
LW	 0.7860	 0.3220
LX	 0.8210	 0.4320
LY	 0.8500	 0.4500
LZ	 0.8320	 0.4090
La	 0.8350	 0.3670
Lb	 0.8310	 0.3800
Lc	 0.8660	 0.4240
Ld	 0.8520	 0.3950
Le	 0.8040	 0.3710
Lf	 0.8120	 0.4100
Lg	 0.8670	 0.4440























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Chain	Atom inclusion	Q-score
Lh	 0.8840	 0.4680
Li	 0.8060	 0.4110
Lj	 0.8220	 0.3790
Lk	 0.8090	 0.3610
Ll	 0.8950	 0.4670
Lm	 0.7860	 0.3300
Ln	 0.8750	 0.4410
Lo	 0.8260	 0.3990
Lp	 0.8030	 0.4130
Lq	 0.8350	 0.4320
Lr	 0.8280	 0.4270
Ls	 0.6430	 0.3290
Lt	 0.8380	 0.2970
S2	 0.9020	 0.3700
SA	 0.6950	 0.3000
SB	 0.6820	 0.2860
SC	 0.6760	 0.2400
SD	 0.5780	 0.1730
SE	 0.7390	 0.2740
SF	 0.7310	 0.3150
SG	 0.6800	 0.2890
SH	 0.7010	 0.2750
SI	 0.6770	 0.2650
SJ	 0.7050	 0.2900
SK	 0.6080	 0.2620
SL	 0.6960	 0.3260
SM	 0.7850	 0.3670
SN	 0.5750	 0.1420
SO	 0.6180	 0.2390
SP	 0.7100	 0.3030
SQ	 0.6700	 0.3000
SR	 0.7780	 0.3720
SS	 0.7970	 0.3580
ST	 0.7680	 0.3090
SU	 0.6480	 0.2620
SV	 0.8290	 0.3660
SW	 0.7500	 0.3100
SX	 0.7890	 0.3990
SY	 0.7630	 0.3580
SZ	 0.7420	 0.3590
Sa	 0.7410	 0.3490
Sb	 0.8140	 0.3970

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Chain	Atom inclusion	Q-score
Sc	 0.8090	 0.4200
Sd	 0.7740	 0.3140
Se	 0.8140	 0.3980
Sf	 0.7390	 0.3380
Sg	 0.7490	 0.3190
Sl	 0.9470	 0.4400
Sm	 0.8870	 0.3140
Sn	 0.8950	 0.3330
So	 0.5370	 0.2640
Sp	 0.7580	 0.2700