



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 08:12 am GMT

PDB ID : 6S05
EMDB ID : EMD-10071
Title : Cryo-EM structures of Lsg1-TAP pre-60S ribosomal particles
Authors : Kargas, V.; Warren, A.J.
Deposited on : 2019-06-13
Resolution : 3.90 Å (reported)
Based on initial model : 4V88

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

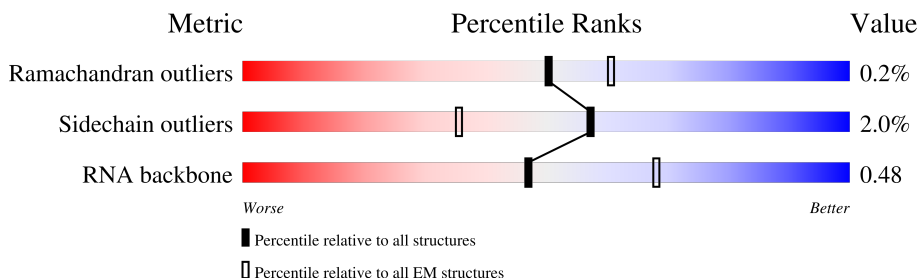
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	3396	
2	B	254	
3	C	387	
4	D	362	
5	E	174	
6	F	191	
7	G	176	
8	H	256	

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Mol	Chain	Length	Quality of chain
9	J	198	6% 99%
10	K	199	9% 93% 7%
11	L	137	8% 98%
12	M	138	8% 97%
13	N	149	99%
14	O	204	100%
15	P	297	8% 91% 9%
16	Q	186	99%
17	R	189	79% 21%
18	S	172	99%
19	T	160	9% 98%
20	U	184	83% 16%
21	V	121	7% 82% 18%
22	W	142	6% 83% 15%
23	X	127	5% 98%
24	Y	136	10% 99%
25	Z	120	98%
26	a	59	8% 88% 12%
27	b	244	89% 10%
28	c	105	12% 92% 8%
29	d	113	10% 95% 5%
30	e	130	5% 94%
31	f	107	6% 97%
32	g	121	5% 83% 15%
33	h	100	29% 97%

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Mol	Chain	Length	Quality of chain
34	i	88	 5% 93% 5%
35	j	78	 12% 96%
36	k	51	 94%
37	l	106	 6% 86% 11%
38	m	92	 9% 92%
39	n	245	 20% 90% 9%
40	z	432	 10% 13% 87%
41	w	518	 40% 71% 25%
42	v	155	 12% 36% 61%
43	o	640	 47% 45% 5% 50%
44	p	210	 54% 100%
45	s	364	 35% 31% 65%
46	x	121	 72% 27%
47	y	158	 75% 23%

2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 129144 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 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	3146	67292	30062	12142	21944	3144	0	0

- Molecule 2 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	247	1878	1170	381	326	1	0	0

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	381	3039	1928	577	526	8	0	0

- Molecule 4 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	361	2748	1730	522	493	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	169	1352	847	253	248	4	0	0

- Molecule 6 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	189	1502	953	272	273	4	0	0

- Molecule 7 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	175	1399	902	251	245	1	0	0

- Molecule 8 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	223	1742	1117	309	313	3	0	0

- Molecule 9 is a protein called 60S ribosomal protein L16-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	197	1563	1005	292	265	1	0	0

- Molecule 10 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	K	186	1486	929	304	253	0	0

- Molecule 11 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	136	1002	628	189	178	7	0	0

- Molecule 12 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	135	1045	669	197	177	2	0	0

- Molecule 13 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	148	1172	749	231	189	3	0	0

- Molecule 14 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	203	Total	C	N	O	S	0	0
			1719	1077	361	280	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	269	Total	C	N	O	S	0	0
			2176	1378	375	421	2		

- Molecule 16 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	185	Total	C	N	O	S	0	0
			1440	908	290	240	2		

- Molecule 17 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	150	Total	C	N	O	0	0
			1209	752	257	200		

- Molecule 18 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	171	Total	C	N	O	S	0	0
			1436	925	266	242	3		

- Molecule 19 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1275	805	246	220	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
20	U	154	Total	C	N	O	0	0
			1222	761	237	224		

- Molecule 21 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	99	Total	C	N	O	0	0
			786	510	129	147		

- Molecule 22 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	120	Total	C	N	O	S	0	0
			958	617	168	171	2		

- Molecule 23 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 24 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	135	Total	C	N	O	0	0
			1091	710	202	179		

- Molecule 25 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	118	Total	C	N	O	S	0	0
			963	612	185	165	1		

- Molecule 26 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	a	52	Total	C	N	O	0	0
			415	259	90	66		

- Molecule 27 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	219	Total	C	N	O	S	0	0
			1760	1138	320	301	1		

- Molecule 28 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	97	Total	C	N	O	S	0	0
			741	479	124	137	1		

- Molecule 29 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	107	Total	C	N	O	S	0	0
			872	553	165	153	1		

- Molecule 30 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	127	Total	C	N	O	S	0	0
			1020	646	205	167	2		

- Molecule 31 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	106	Total	C	N	O	S	0	0
			849	540	165	143	1		

- Molecule 32 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	103	Total	C	N	O	S	0	0
			812	504	167	137	4		

- Molecule 33 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	98	Total	C	N	O	S	0	0
			763	477	155	129	2		

- Molecule 34 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 35 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	j	77	Total	C	N	O	0	0
			611	391	115	105		

- Molecule 36 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	50	Total	C	N	O	S	0	0
			435	272	97	64	2		

- Molecule 37 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	94	Total	C	N	O	S	0	0
			756	476	153	122	5		

- Molecule 38 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	89	Total	C	N	O	S	0	0
			680	421	136	117	6		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	224	Total	C	N	O	S	0	0
			1691	1051	293	340	7		

- Molecule 40 is a protein called Cytoplasmic 60S subunit biogenesis factor REH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	z	58	Total	C	N	O	S	0	0
			491	301	100	87	3		

- Molecule 41 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	389	Total	C	N	O	S	0	0
			3076	1955	530	571	20		

- Molecule 42 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	v	60	Total	C	N	O	S	0	0
			500	322	98	79	1		

- Molecule 43 is a protein called Large subunit GTPase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	322	Total	C	N	O	S	0	0
			2593	1660	449	477	7		

- Molecule 44 is a protein called uL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	p	210	Total	C	N	O	0	0
			1050	630	210	210		

- Molecule 45 is a protein called Tyrosine-protein phosphatase YVH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	128	Total	C	N	O	S	0	0
			991	625	179	179	8		

- Molecule 46 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	x	121	Total	C	N	O	P	0	0
			2576	1152	461	843	120		

- Molecule 47 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	y	156	Total	C	N	O	P	0	0
			3310	1482	582	1091	155		

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
48	g	1	Total	Zn	0
			1	1	
48	i	1	Total	Zn	0
			1	1	
48	l	1	Total	Zn	0
			1	1	

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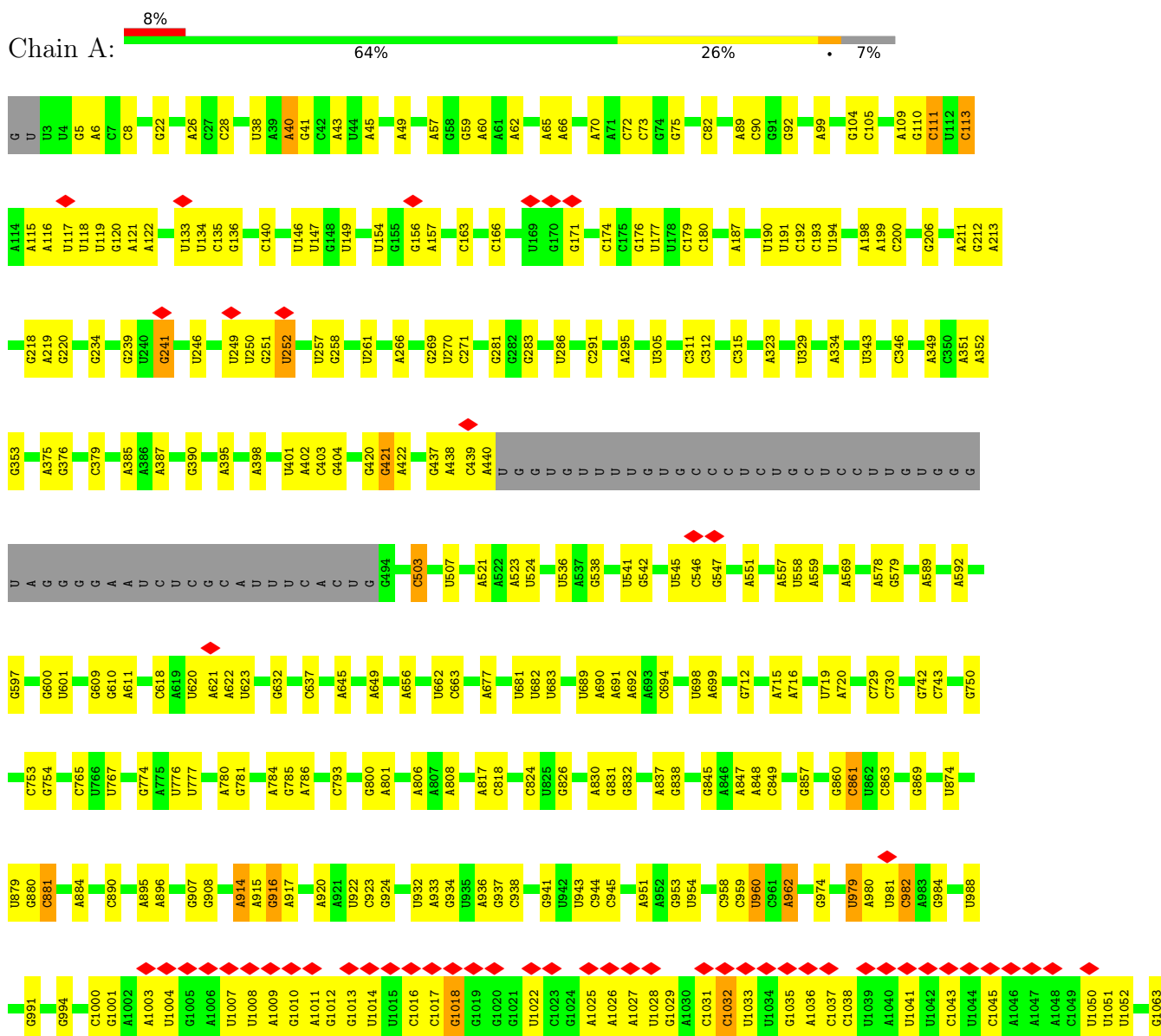
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Mol	Chain	Residues	Atoms		AltConf
48	m	1	Total 1	Zn 1	0
48	w	2	Total 2	Zn 2	0
48	s	2	Total 2	Zn 2	0

3 Residue-property plots i

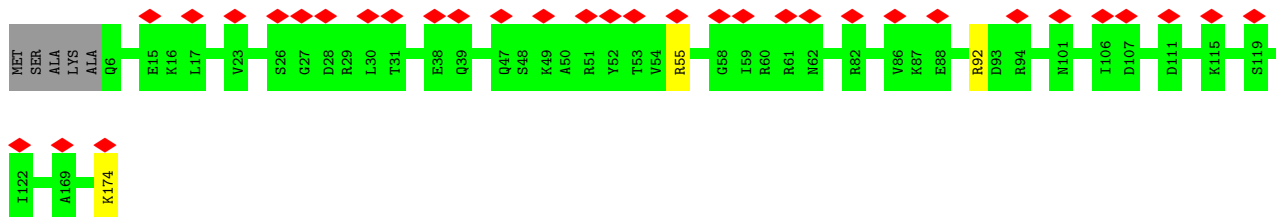
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 25S ribosomal RNA

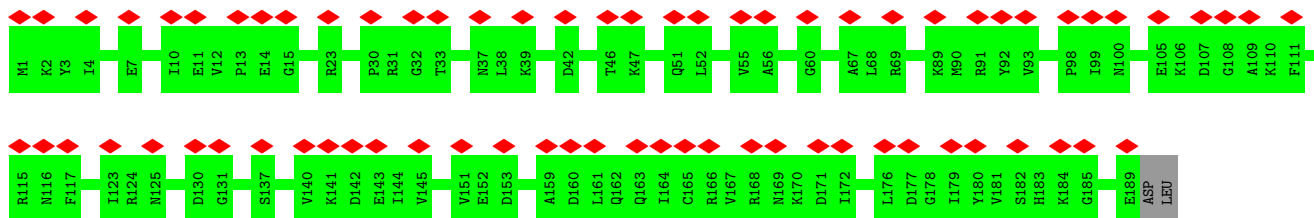




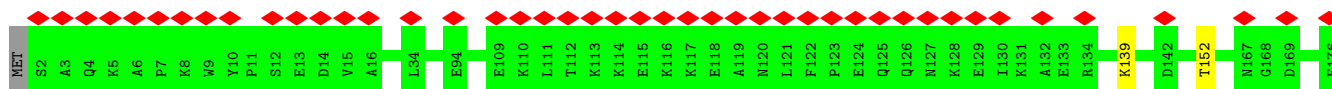
• Molecule 5: 60S ribosomal protein L11-A



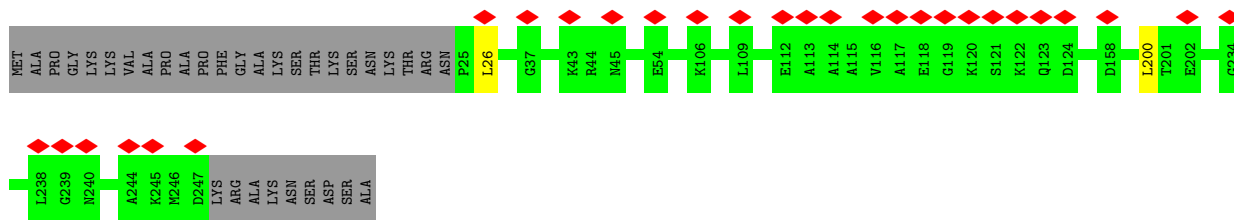
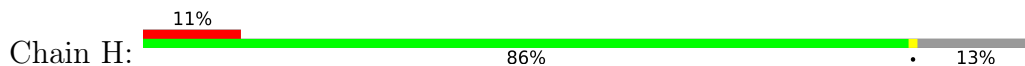
• Molecule 6: 60S ribosomal protein L9-A



• Molecule 7: 60S ribosomal protein L6-A

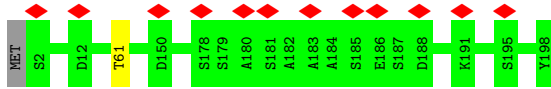


• Molecule 8: 60S ribosomal protein L8-A

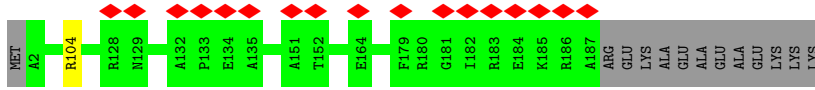
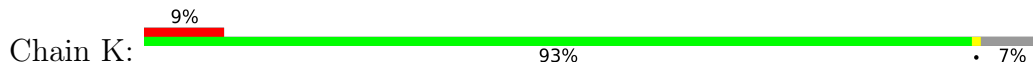


• Molecule 9: 60S ribosomal protein L16-B

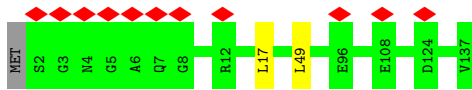




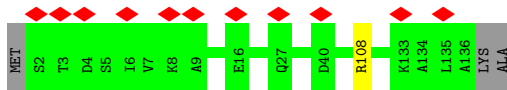
- Molecule 10: 60S ribosomal protein L13-A



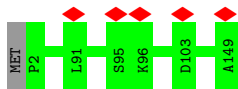
- Molecule 11: 60S ribosomal protein L23-A



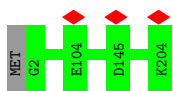
- Molecule 12: 60S ribosomal protein L14-A



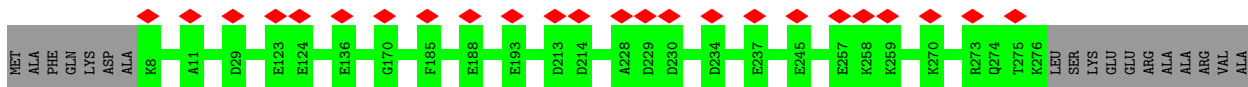
- Molecule 13: 60S ribosomal protein L28



- Molecule 14: 60S ribosomal protein L15-A



- Molecule 15: 60S ribosomal protein L5




ALA
LYS
ILE
ALA
LEU
ALA
GLY
GLN

- Molecule 16: 60S ribosomal protein L18-A

Chain Q:  99%

MET
G2
I3
D4
S13
D41
D125
E148
Y186

- Molecule 17: 60S ribosomal protein L19-A

Chain R:  79% 21%

MET
A2
A112
D148
A149
Q150
R151
GLU
LYS
ALA
LEU
ASN
GLU
GLU
ALA
ALA
ALA
ARG
ARG
LEU
LYS
ASN
ARG
ALA
ALA
ARG
ASP
ARG
ALA
GLN
ARG
VAL
ALA
GLU
LYS
ARG
ASP
ALA
LEU
LEU
LYS
GLU
ASP
ALA

- Molecule 18: 60S ribosomal protein L20-A

Chain S:  99%


MET
A2
S18
D62
S83
R94
D96
D134
K146
D147
Y172

- Molecule 19: 60S ribosomal protein L21-A

Chain T:  9% 98%

MET
G2
K3
D38
R83
M112
A117
A121
Q122
G123
V124
R136
E137
L151
Y156
E157
T158
F159
I160

- Molecule 20: 60S ribosomal protein L17-A

Chain U:  83% 16%

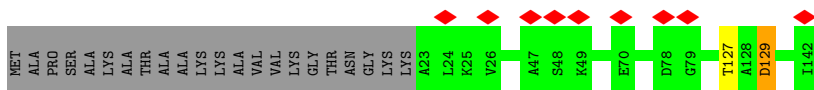
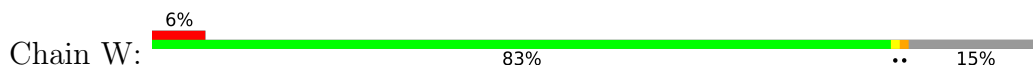
MET
A2
K138
E154
E155
ALA
VAL
ALA
LYS
ALA
ALA
GLU
LYS
VAL
VAL
ARG
LEU
THR
SER
ARG
GLN
ARG
GLY
ARG
ILE
ALA
ALA
GLN
LYS
ARG
ILE
ALA
ALA

- Molecule 21: 60S ribosomal protein L22-A

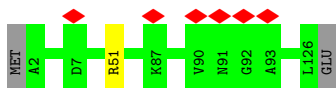
Chain V: 7% 82% 18%

MET
ALA
PRO
ASN
THR
SER
ARG
LYS
GLN
LYS
I11
E24
A31
L50
G51
N52
E58
D59
G60
Q109
VAL
THR
PRO
GLU
GLU
GLU
ASP
GLU
GLU
ASP
GLU
GLU

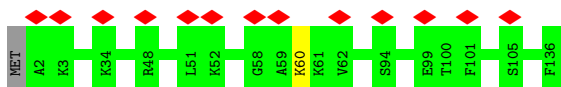
- Molecule 22: 60S ribosomal protein L25



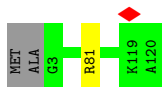
- Molecule 23: 60S ribosomal protein L26-A



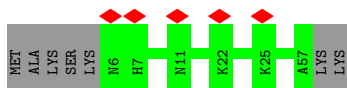
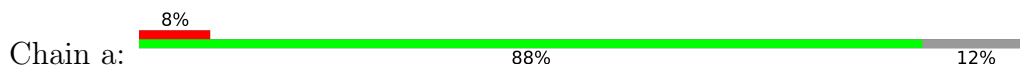
- Molecule 24: 60S ribosomal protein L27-A



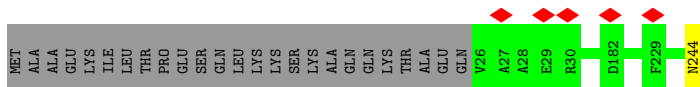
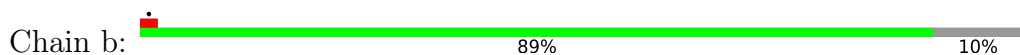
- Molecule 25: 60S ribosomal protein L35-A



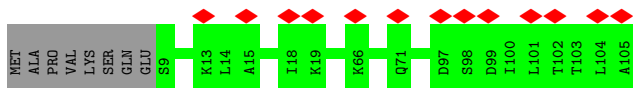
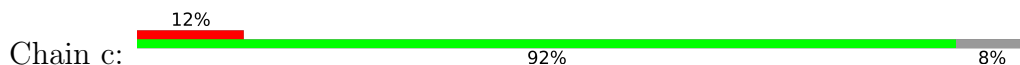
- Molecule 26: 60S ribosomal protein L29



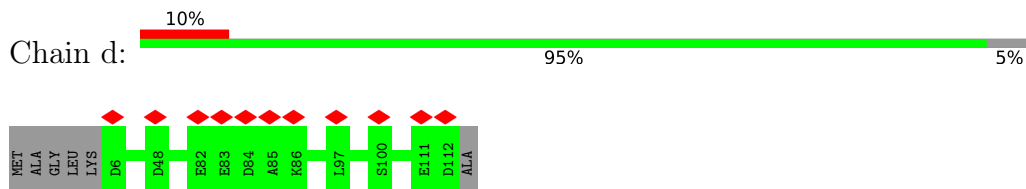
- Molecule 27: 60S ribosomal protein L7-A



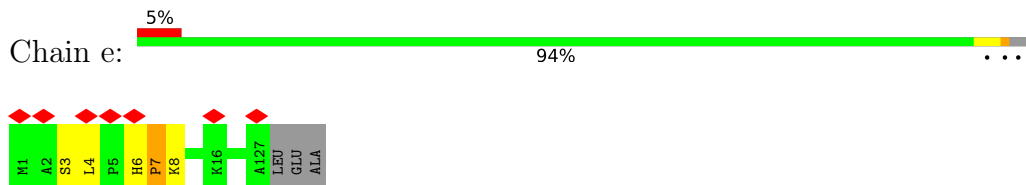
- Molecule 28: 60S ribosomal protein L30



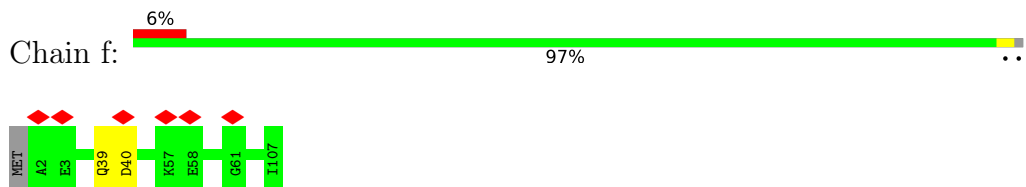
- Molecule 29: 60S ribosomal protein L31-A



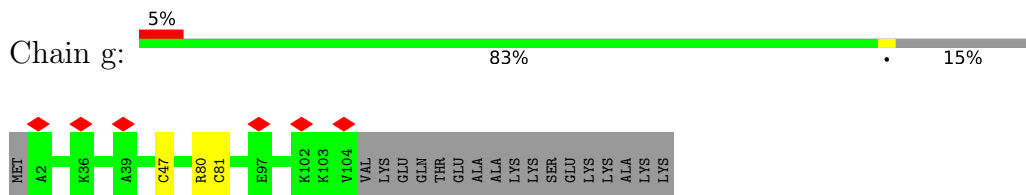
- Molecule 30: 60S ribosomal protein L32



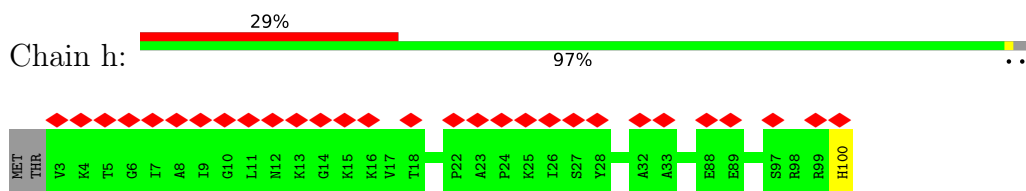
- Molecule 31: 60S ribosomal protein L33-A



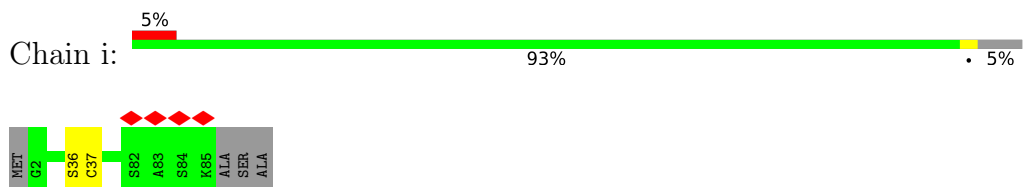
- Molecule 32: 60S ribosomal protein L34-A



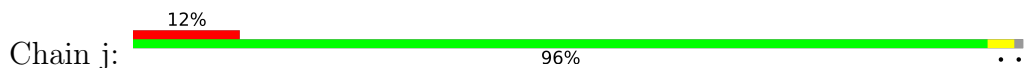
- Molecule 33: 60S ribosomal protein L36-A



- Molecule 34: 60S ribosomal protein L37-A



- Molecule 35: 60S ribosomal protein L38



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35152	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.460	Depositor
Minimum map value	-0.235	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.08	Depositor
Map size (\AA)	383.40002, 383.40002, 383.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.065, 1.065, 1.065	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.89	3/75327 (0.0%)	1.20	505/117440 (0.4%)
2	B	0.50	0/1912	0.62	0/2569
3	C	0.50	0/3110	0.60	1/4184 (0.0%)
4	D	0.48	0/2800	0.59	1/3791 (0.0%)
5	E	0.33	0/1373	0.59	0/1841
6	F	0.33	0/1523	0.58	0/2051
7	G	0.37	0/1423	0.57	0/1911
8	H	0.41	0/1774	0.58	2/2395 (0.1%)
9	J	0.46	0/1593	0.56	0/2137
10	K	0.46	0/1511	0.56	0/2031
11	L	0.43	0/1017	0.61	1/1368 (0.1%)
12	M	0.40	0/1060	0.60	0/1428
13	N	0.48	0/1203	0.60	0/1611
14	O	0.54	0/1756	0.58	0/2353
15	P	0.41	0/2225	0.57	0/3004
16	Q	0.46	0/1464	0.54	0/1964
17	R	0.43	0/1226	0.54	0/1637
18	S	0.46	0/1472	0.58	0/1979
19	T	0.45	0/1299	0.54	0/1742
20	U	0.52	0/1245	0.57	0/1676
21	V	0.40	0/802	0.62	0/1087
22	W	0.47	0/973	0.65	1/1313 (0.1%)
23	X	0.45	0/995	0.58	0/1329
24	Y	0.38	0/1117	0.53	0/1496
25	Z	0.42	0/972	0.52	0/1293
26	a	0.33	0/426	0.52	0/570
27	b	0.51	0/1797	0.59	0/2419
28	c	0.40	0/749	0.54	0/1007
29	d	0.50	0/886	0.66	0/1190
30	e	0.48	0/1041	0.61	1/1393 (0.1%)
31	f	0.54	0/867	0.71	2/1167 (0.2%)
32	g	0.46	0/822	0.59	0/1099

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.36	0/770	0.52	0/1023
34	i	0.52	0/680	0.63	0/901
35	j	0.38	0/617	0.57	0/825
36	k	0.45	0/442	0.52	0/587
37	l	0.47	0/768	0.66	0/1016
38	m	0.43	0/687	0.59	0/915
39	n	0.34	0/1712	0.58	0/2330
40	z	0.31	0/494	0.57	0/654
41	w	0.58	6/3135 (0.2%)	0.70	3/4255 (0.1%)
42	v	0.38	0/512	0.55	0/680
43	o	0.50	3/2647 (0.1%)	0.73	2/3582 (0.1%)
45	s	0.51	1/1016 (0.1%)	0.88	4/1368 (0.3%)
46	x	0.75	0/2880	1.11	14/4487 (0.3%)
47	y	0.96	0/3699	1.18	21/5760 (0.4%)
All	All	0.74	13/137819 (0.0%)	1.02	558/202858 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	w	25	PRO	N-CA	13.75	1.70	1.47
41	w	298	PRO	N-CA	12.89	1.69	1.47
45	s	307	CYS	C-N	8.83	1.51	1.34
41	w	143	CYS	C-N	8.80	1.50	1.34
41	w	249	VAL	C-N	8.77	1.50	1.34
43	o	409	LEU	C-N	8.70	1.50	1.34
43	o	367	THR	C-N	8.62	1.50	1.34
43	o	179	THR	C-N	8.54	1.50	1.34
1	A	2258	U	C1'-N1	6.03	1.57	1.48
41	w	297	SER	C-N	5.79	1.45	1.34
41	w	24	THR	C-N	5.54	1.44	1.34
1	A	656	A	N7-C5	-5.50	1.35	1.39
1	A	914	A	N9-C4	-5.21	1.34	1.37

All (558) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	s	247	ALA	CB-CA-C	-12.41	91.49	110.10
1	A	3092	C	N1-C2-O2	11.55	125.83	118.90
1	A	945	C	C6-N1-C2	-11.36	115.76	120.30
1	A	3092	C	C2-N1-C1'	10.61	130.47	118.80
45	s	248	HIS	N-CA-CB	-10.48	91.73	110.60
1	A	252	U	C2-N1-C1'	10.44	130.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	s	247	ALA	N-CA-C	-10.14	83.63	111.00
46	x	105	C	N1-C2-O2	10.12	124.97	118.90
1	A	1279	C	C5-C6-N1	9.91	125.96	121.00
1	A	252	U	N3-C2-O2	-9.82	115.33	122.20
1	A	1496	C	C2-N1-C1'	9.79	129.57	118.80
1	A	252	U	N1-C2-O2	9.69	129.59	122.80
47	y	135	G	N3-C4-N9	-9.49	120.31	126.00
1	A	922	U	C2-N1-C1'	9.49	129.09	117.70
1	A	2506	U	N3-C2-O2	-9.34	115.66	122.20
1	A	1279	C	C6-N1-C2	-9.33	116.57	120.30
1	A	2567	C	N3-C2-O2	-9.24	115.43	121.90
1	A	2983	C	N3-C2-O2	-9.18	115.48	121.90
1	A	3181	C	N1-C2-O2	9.04	124.32	118.90
1	A	3092	C	N3-C2-O2	-9.03	115.58	121.90
1	A	1496	C	N1-C2-O2	9.01	124.30	118.90
1	A	1907	C	N1-C2-O2	8.94	124.27	118.90
1	A	2137	U	N3-C2-O2	-8.84	116.01	122.20
1	A	2552	C	C2-N1-C1'	8.74	128.42	118.80
41	w	298	PRO	CA-N-CD	-8.73	99.28	111.50
1	A	2132	C	N3-C2-O2	-8.71	115.80	121.90
1	A	3181	C	C2-N1-C1'	8.69	128.36	118.80
1	A	1283	C	N3-C2-O2	-8.56	115.91	121.90
1	A	241	G	C4-N9-C1'	8.53	137.59	126.50
46	x	105	C	C2-N1-C1'	8.49	128.14	118.80
1	A	2983	C	N1-C2-O2	8.46	123.97	118.90
1	A	3104	U	N1-C2-O2	8.44	128.71	122.80
1	A	2928	C	C6-N1-C2	-8.44	116.92	120.30
1	A	2983	C	C2-N1-C1'	8.40	128.04	118.80
1	A	1269	U	C2-N1-C1'	8.40	127.78	117.70
1	A	3105	U	C2-N1-C1'	8.39	127.77	117.70
1	A	663	C	C5-C6-N1	8.38	125.19	121.00
1	A	3104	U	N3-C2-O2	-8.37	116.34	122.20
31	f	40	ASP	CB-CG-OD1	8.34	125.81	118.30
1	A	2434	U	C2-N1-C1'	8.29	127.65	117.70
46	x	105	C	N3-C2-O2	-8.26	116.12	121.90
1	A	2137	U	N1-C2-O2	8.24	128.57	122.80
4	D	349	THR	C-N-CA	8.22	142.25	121.70
1	A	2552	C	N1-C2-O2	8.18	123.81	118.90
1	A	2366	C	C6-N1-C2	-8.15	117.04	120.30
1	A	2783	U	N3-C2-O2	-8.14	116.50	122.20
1	A	1872	C	N1-C2-O2	8.13	123.78	118.90
1	A	105	C	C6-N1-C2	-8.07	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2434	U	N3-C2-O2	-8.06	116.56	122.20
1	A	149	U	N3-C2-O2	-8.04	116.57	122.20
1	A	1762	C	C6-N1-C2	-8.02	117.09	120.30
1	A	743	C	N1-C2-O2	8.02	123.71	118.90
1	A	2638	C	N1-C2-O2	7.97	123.69	118.90
1	A	2434	U	N1-C2-O2	7.89	128.32	122.80
1	A	1283	C	N1-C2-O2	7.85	123.61	118.90
1	A	3181	C	N3-C2-O2	-7.84	116.41	121.90
1	A	2263	C	C2-N1-C1'	7.83	127.41	118.80
1	A	3092	C	C6-N1-C1'	-7.83	111.41	120.80
1	A	922	U	N3-C2-O2	-7.80	116.74	122.20
1	A	2434	U	C5-C6-N1	7.80	126.60	122.70
1	A	524	U	N3-C2-O2	-7.75	116.77	122.20
1	A	3104	U	C2-N1-C1'	7.65	126.88	117.70
1	A	2132	C	N1-C2-O2	7.64	123.48	118.90
1	A	2506	U	N1-C2-O2	7.63	128.14	122.80
47	y	113	U	C2-N1-C1'	7.60	126.82	117.70
1	A	1872	C	C6-N1-C2	-7.60	117.26	120.30
1	A	945	C	N1-C2-N3	7.59	124.51	119.20
1	A	1710	C	C6-N1-C2	-7.51	117.29	120.30
1	A	524	U	N1-C2-O2	7.51	128.05	122.80
46	x	105	C	C6-N1-C2	-7.42	117.33	120.30
3	C	18	PRO	CA-N-CD	-7.42	101.11	111.50
1	A	2196	C	C6-N1-C2	-7.42	117.33	120.30
1	A	271	C	N3-C2-O2	-7.38	116.73	121.90
1	A	922	U	N1-C2-O2	7.37	127.96	122.80
1	A	241	G	N3-C4-C5	-7.34	124.93	128.60
1	A	1496	C	N3-C2-O2	-7.34	116.76	121.90
1	A	1907	C	N3-C2-O2	-7.33	116.77	121.90
1	A	2366	C	N3-C2-O2	-7.26	116.82	121.90
1	A	1031	C	C2-N1-C1'	7.25	126.78	118.80
1	A	960	U	C2-N1-C1'	7.24	126.39	117.70
1	A	2980	U	N3-C2-O2	-7.23	117.14	122.20
1	A	3105	U	N1-C2-O2	7.23	127.86	122.80
22	W	129	ASP	CB-CA-C	-7.22	95.97	110.40
47	y	135	G	C5-C6-O6	7.22	132.93	128.60
1	A	105	C	C2-N1-C1'	7.19	126.71	118.80
1	A	2567	C	N1-C2-O2	7.18	123.21	118.90
1	A	1269	U	N1-C2-O2	7.17	127.82	122.80
1	A	1227	C	N1-C2-O2	7.14	123.18	118.90
1	A	271	C	N1-C2-O2	7.13	123.18	118.90
1	A	241	G	N3-C4-N9	7.09	130.25	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2737	C	N1-C2-O2	7.08	123.15	118.90
1	A	113	C	N1-C2-O2	7.07	123.14	118.90
1	A	1279	C	N1-C2-O2	7.07	123.14	118.90
1	A	1496	C	C6-N1-C1'	-7.06	112.33	120.80
1	A	1031	C	N1-C2-O2	7.05	123.13	118.90
1	A	1907	C	C2-N1-C1'	6.99	126.49	118.80
1	A	1239	C	N1-C2-O2	6.98	123.09	118.90
1	A	2622	C	N1-C2-O2	6.97	123.08	118.90
1	A	2567	C	C6-N1-C2	-6.97	117.51	120.30
1	A	2638	C	N3-C2-O2	-6.95	117.03	121.90
1	A	3105	U	N3-C2-O2	-6.95	117.33	122.20
1	A	2551	U	C2-N1-C1'	6.95	126.04	117.70
1	A	1781	C	C6-N1-C2	-6.94	117.52	120.30
1	A	2137	U	C2-N1-C1'	6.94	126.03	117.70
1	A	2954	U	N1-C2-O2	6.94	127.66	122.80
1	A	2594	C	N1-C2-O2	6.93	123.06	118.90
1	A	2681	U	C5-C6-N1	6.88	126.14	122.70
1	A	2101	C	P-O3'-C3'	6.88	127.95	119.70
1	A	261	U	N1-C2-O2	6.87	127.61	122.80
1	A	241	G	C8-N9-C1'	-6.86	118.08	127.00
1	A	663	C	C6-N1-C2	-6.86	117.56	120.30
1	A	881	C	N1-C2-O2	6.84	123.00	118.90
1	A	503	C	C6-N1-C2	-6.83	117.57	120.30
1	A	1815	U	P-O3'-C3'	6.83	127.90	119.70
1	A	105	C	C5-C6-N1	6.82	124.41	121.00
1	A	2928	C	C2-N1-C1'	6.80	126.28	118.80
1	A	2497	U	N1-C2-O2	6.79	127.56	122.80
47	y	102	U	C2-N1-C1'	6.77	125.82	117.70
1	A	2112	U	P-O3'-C3'	6.73	127.78	119.70
1	A	1854	C	N1-C2-O2	6.73	122.94	118.90
1	A	1872	C	N3-C2-O2	-6.72	117.19	121.90
47	y	119	C	N3-C2-O2	-6.72	117.19	121.90
1	A	1493	G	C4-N9-C1'	6.71	135.23	126.50
1	A	1255	C	N1-C2-O2	6.71	122.93	118.90
1	A	1525	G	C4-N9-C1'	6.71	135.22	126.50
1	A	1710	C	C2-N1-C1'	6.71	126.17	118.80
1	A	2729	U	N3-C2-O2	-6.70	117.51	122.20
1	A	2552	C	C6-N1-C1'	-6.70	112.76	120.80
1	A	2264	U	N1-C2-O2	6.70	127.49	122.80
1	A	3105	U	C5-C6-N1	6.70	126.05	122.70
1	A	793	C	C5-C6-N1	6.69	124.35	121.00
1	A	2980	U	N1-C2-O2	6.68	127.48	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2681	U	C2-N1-C1'	6.67	125.70	117.70
41	w	25	PRO	CA-N-CD	-6.65	102.19	111.50
1	A	682	U	N3-C2-O2	-6.64	117.55	122.20
1	A	2132	C	C6-N1-C2	-6.63	117.65	120.30
1	A	2600	C	C6-N1-C2	-6.63	117.65	120.30
1	A	2737	C	N3-C2-O2	-6.63	117.26	121.90
1	A	2560	C	C6-N1-C2	-6.61	117.66	120.30
1	A	1437	C	C6-N1-C2	-6.59	117.66	120.30
1	A	1872	C	C5-C6-N1	6.59	124.30	121.00
1	A	1312	C	C6-N1-C2	-6.58	117.67	120.30
1	A	1943	C	N1-C2-O2	6.57	122.84	118.90
1	A	252	U	C6-N1-C1'	-6.56	112.01	121.20
1	A	3298	C	C6-N1-C2	-6.56	117.67	120.30
1	A	2506	U	C2-N1-C1'	6.55	125.56	117.70
1	A	2849	C	C6-N1-C2	-6.55	117.68	120.30
1	A	113	C	C2-N1-C1'	6.53	125.99	118.80
1	A	2954	U	N3-C2-O2	-6.52	117.64	122.20
1	A	2783	U	N1-C2-O2	6.51	127.36	122.80
1	A	3181	C	C6-N1-C2	-6.50	117.70	120.30
1	A	1216	C	N1-C2-O2	6.48	122.79	118.90
1	A	2497	U	N3-C2-O2	-6.47	117.67	122.20
1	A	2737	C	C6-N1-C2	-6.47	117.71	120.30
1	A	1522	U	C5-C6-N1	-6.46	119.47	122.70
47	y	113	U	N1-C2-O2	6.45	127.32	122.80
1	A	1276	U	C2-N1-C1'	6.45	125.44	117.70
1	A	3131	U	N1-C2-O2	6.44	127.31	122.80
1	A	3131	U	N3-C2-O2	-6.43	117.70	122.20
1	A	800	G	C4-N9-C1'	6.43	134.86	126.50
1	A	682	U	N1-C2-O2	6.42	127.30	122.80
1	A	3153	U	N1-C2-O2	6.41	127.29	122.80
1	A	682	U	C2-N1-C1'	6.40	125.38	117.70
1	A	2928	C	C5-C6-N1	6.40	124.20	121.00
1	A	1267	U	N1-C2-O2	6.40	127.28	122.80
8	H	26	LEU	CA-CB-CG	6.39	129.99	115.30
1	A	2849	C	N1-C2-O2	6.37	122.72	118.90
1	A	3153	U	N3-C2-O2	-6.37	117.74	122.20
47	y	135	G	N3-C4-C5	6.37	131.78	128.60
1	A	1353	U	N1-C2-O2	6.36	127.25	122.80
1	A	1353	U	C2-N1-C1'	6.34	125.31	117.70
1	A	2434	U	C6-N1-C2	-6.34	117.19	121.00
41	w	89	LEU	CA-CB-CG	6.34	129.88	115.30
1	A	945	C	N3-C2-O2	-6.34	117.46	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	y	64	U	N3-C2-O2	-6.33	117.77	122.20
1	A	1353	U	C5-C6-N1	6.33	125.86	122.70
46	x	105	C	C5-C6-N1	6.32	124.16	121.00
1	A	2420	C	C5-C6-N1	6.31	124.15	121.00
1	A	2550	U	N3-C2-O2	-6.29	117.80	122.20
1	A	2899	C	C2-N1-C1'	6.28	125.71	118.80
47	y	102	U	N3-C2-O2	-6.28	117.81	122.20
47	y	135	G	N9-C4-C5	6.27	107.91	105.40
1	A	1276	U	N3-C2-O2	-6.27	117.81	122.20
1	A	1276	U	N1-C2-O2	6.26	127.18	122.80
1	A	2274	U	C2-N1-C1'	6.26	125.21	117.70
1	A	2638	C	C2-N1-C1'	6.26	125.68	118.80
1	A	1943	C	N3-C2-O2	-6.25	117.53	121.90
1	A	283	G	C4-N9-C1'	6.25	134.62	126.50
1	A	2551	U	N1-C2-O2	6.24	127.17	122.80
1	A	1878	G	C4-N9-C1'	6.24	134.60	126.50
1	A	2954	U	C2-N1-C1'	6.23	125.18	117.70
1	A	2263	C	C6-N1-C2	-6.23	117.81	120.30
47	y	142	C	C6-N1-C2	-6.22	117.81	120.30
1	A	2773	C	C6-N1-C2	-6.22	117.81	120.30
1	A	2983	C	C6-N1-C2	-6.22	117.81	120.30
1	A	3034	C	N1-C2-O2	6.21	122.63	118.90
1	A	1269	U	N3-C2-O2	-6.21	117.85	122.20
1	A	1743	G	C4-N9-C1'	6.21	134.57	126.50
1	A	1255	C	N3-C2-O2	-6.20	117.56	121.90
1	A	2500	A	C8-N9-C4	-6.20	103.32	105.80
1	A	2331	C	N1-C2-O2	6.19	122.61	118.90
1	A	1604	G	N3-C4-N9	6.19	129.71	126.00
1	A	934	G	C4-N9-C1'	6.19	134.54	126.50
1	A	1854	C	C2-N1-C1'	6.18	125.60	118.80
1	A	988	U	C5-C6-N1	6.17	125.79	122.70
1	A	1224	C	N1-C2-O2	6.17	122.60	118.90
1	A	2581	U	N3-C2-O2	-6.17	117.88	122.20
1	A	1064	A	P-O3'-C3'	6.16	127.09	119.70
1	A	1493	G	N3-C4-N9	6.16	129.70	126.00
1	A	2264	U	N3-C2-O2	-6.16	117.89	122.20
1	A	1854	C	C6-N1-C2	-6.16	117.84	120.30
1	A	2209	U	C2-N1-C1'	6.15	125.08	117.70
1	A	1493	G	C8-N9-C1'	-6.15	119.01	127.00
1	A	743	C	N3-C2-O2	-6.14	117.60	121.90
1	A	3214	U	C2-N1-C1'	6.14	125.07	117.70
1	A	2596	U	N3-C2-O2	-6.14	117.90	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1275	C	N1-C2-O2	6.13	122.58	118.90
1	A	40	A	O4'-C1'-N9	6.12	113.09	108.20
1	A	1872	C	C2-N1-C1'	6.12	125.53	118.80
1	A	1843	C	C6-N1-C2	-6.11	117.86	120.30
1	A	958	C	N3-C2-O2	-6.10	117.63	121.90
1	A	2600	C	N1-C2-O2	6.09	122.55	118.90
1	A	3141	A	N1-C6-N6	6.09	122.25	118.60
1	A	1496	C	C6-N1-C2	-6.09	117.86	120.30
1	A	3161	C	N1-C2-O2	6.08	122.55	118.90
1	A	1238	C	N1-C2-O2	6.08	122.55	118.90
1	A	1333	C	C6-N1-C2	-6.07	117.87	120.30
1	A	2594	C	N3-C2-O2	-6.07	117.65	121.90
1	A	2305	G	N3-C4-C5	-6.07	125.56	128.60
1	A	2365	C	N1-C2-O2	6.06	122.53	118.90
1	A	2407	C	C6-N1-C2	-6.05	117.88	120.30
1	A	1710	C	N1-C2-O2	6.03	122.52	118.90
11	L	17	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	861	C	C2-N1-C1'	6.02	125.42	118.80
47	y	119	C	C6-N1-C2	-6.02	117.89	120.30
1	A	2153	U	N3-C2-O2	-6.01	118.00	122.20
1	A	1437	C	C5-C6-N1	6.00	124.00	121.00
1	A	2196	C	C5-C6-N1	5.99	123.99	121.00
1	A	1267	U	C2-N1-C1'	5.99	124.88	117.70
1	A	379	C	N1-C2-O2	5.98	122.49	118.90
1	A	2600	C	N3-C2-O2	-5.98	117.72	121.90
1	A	1459	C	C6-N1-C2	-5.97	117.91	120.30
1	A	1710	C	C5-C6-N1	5.96	123.98	121.00
1	A	2763	U	C5-C6-N1	5.96	125.68	122.70
1	A	800	G	N3-C4-N9	5.95	129.57	126.00
1	A	2331	C	C6-N1-C2	-5.94	117.92	120.30
1	A	2264	U	C2-N1-C1'	5.94	124.82	117.70
1	A	2560	C	C5-C6-N1	5.93	123.97	121.00
1	A	3324	C	C6-N1-C2	-5.93	117.93	120.30
8	H	200	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	2209	U	N1-C2-O2	5.92	126.94	122.80
1	A	934	G	C8-N9-C1'	-5.92	119.31	127.00
1	A	2815	G	N1-C2-N3	5.92	127.45	123.90
1	A	113	C	N3-C2-O2	-5.91	117.76	121.90
1	A	824	C	C6-N1-C2	-5.91	117.94	120.30
1	A	2764	C	N1-C2-O2	5.90	122.44	118.90
1	A	2755	C	N1-C2-O2	5.90	122.44	118.90
1	A	503	C	C5-C6-N1	5.89	123.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	922	U	C6-N1-C1'	-5.88	112.96	121.20
1	A	1031	C	N3-C2-O2	-5.88	117.78	121.90
1	A	979	U	P-O3'-C3'	5.87	126.75	119.70
1	A	261	U	N3-C2-O2	-5.87	118.09	122.20
1	A	2333	C	C6-N1-C2	-5.86	117.95	120.30
1	A	922	U	C5-C6-N1	5.85	125.63	122.70
1	A	291	C	C6-N1-C2	-5.85	117.96	120.30
1	A	2305	G	N3-C4-N9	5.85	129.51	126.00
1	A	1943	C	C6-N1-C2	-5.85	117.96	120.30
1	A	2265	C	C6-N1-C2	-5.84	117.96	120.30
1	A	2822	U	C5-C6-N1	5.84	125.62	122.70
1	A	1267	U	N3-C2-O2	-5.83	118.12	122.20
1	A	1604	G	C4-N9-C1'	5.83	134.08	126.50
1	A	252	U	C5-C6-N1	5.83	125.61	122.70
1	A	1854	C	N3-C2-O2	-5.83	117.82	121.90
1	A	1299	U	N1-C2-O2	5.82	126.88	122.80
1	A	1571	A	C8-N9-C4	-5.82	103.47	105.80
1	A	2263	C	C5-C6-N1	5.82	123.91	121.00
1	A	1762	C	C5-C6-N1	5.82	123.91	121.00
1	A	945	C	C6-N1-C1'	5.81	127.78	120.80
1	A	1333	C	C2-N1-C1'	5.81	125.19	118.80
1	A	2737	C	C2-N1-C1'	5.81	125.19	118.80
1	A	1639	C	N1-C2-O2	5.80	122.38	118.90
1	A	1843	C	C2-N1-C1'	5.80	125.18	118.80
1	A	1425	U	N3-C2-O2	-5.79	118.14	122.20
1	A	2585	G	N3-C4-C5	-5.79	125.70	128.60
1	A	818	C	C2-N1-C1'	5.78	125.16	118.80
1	A	90	C	C2-N1-C1'	5.77	125.15	118.80
1	A	3181	C	C6-N1-C1'	-5.77	113.88	120.80
1	A	2431	C	C6-N1-C2	-5.76	118.00	120.30
1	A	2497	U	C5-C6-N1	5.76	125.58	122.70
1	A	881	C	N3-C2-O2	-5.75	117.87	121.90
1	A	2420	C	C6-N1-C2	-5.75	118.00	120.30
1	A	2704	A	N1-C6-N6	-5.75	115.15	118.60
45	s	241	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	291	C	C5-C6-N1	5.74	123.87	121.00
1	A	2349	U	C2-N1-C1'	5.73	124.57	117.70
1	A	1889	G	C4-N9-C1'	5.71	133.92	126.50
1	A	2114	C	C6-N1-C2	-5.71	118.02	120.30
1	A	2638	C	C6-N1-C2	-5.70	118.02	120.30
1	A	2566	C	C6-N1-C2	-5.69	118.02	120.30
1	A	1433	A	O4'-C1'-N9	-5.69	103.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	e	7	PRO	N-CA-CB	-5.69	96.34	102.60
1	A	1614	C	C6-N1-C2	-5.69	118.03	120.30
1	A	193	C	C6-N1-C2	-5.69	118.03	120.30
1	A	2263	C	N1-C2-O2	5.69	122.31	118.90
1	A	3153	U	C2-N1-C1'	5.68	124.52	117.70
1	A	1032	C	C5-C6-N1	5.68	123.84	121.00
47	y	28	C	C6-N1-C2	-5.68	118.03	120.30
1	A	1263	A	C2-N3-C4	5.68	113.44	110.60
1	A	1298	C	C6-N1-C2	-5.68	118.03	120.30
1	A	421	G	N3-C4-N9	5.66	129.40	126.00
46	x	50	U	N3-C2-O2	-5.66	118.24	122.20
1	A	8	C	C5-C6-N1	5.66	123.83	121.00
1	A	754	G	C6-C5-N7	-5.66	127.00	130.40
1	A	1827	C	N3-C2-O2	-5.65	117.94	121.90
1	A	2455	U	N1-C2-O2	5.65	126.75	122.80
1	A	2581	U	N1-C2-O2	5.65	126.75	122.80
1	A	1208	U	C5-C6-N1	5.64	125.52	122.70
1	A	421	G	C4-N9-C1'	5.63	133.82	126.50
1	A	2473	C	C5-C6-N1	5.63	123.82	121.00
1	A	2594	C	C2-N1-C1'	5.63	125.00	118.80
1	A	311	C	C2-N1-C1'	5.63	124.99	118.80
1	A	1604	G	C8-N9-C1'	-5.62	119.69	127.00
1	A	2329	C	C6-N1-C2	-5.62	118.05	120.30
1	A	1279	C	N3-C2-O2	-5.62	117.97	121.90
1	A	3265	C	N1-C2-O2	5.62	122.27	118.90
1	A	2585	G	N3-C4-N9	5.62	129.37	126.00
1	A	618	C	C6-N1-C2	-5.61	118.06	120.30
1	A	1493	G	N3-C4-C5	-5.61	125.80	128.60
31	f	39	GLN	C-N-CA	5.60	135.71	121.70
1	A	2596	U	N1-C2-O2	5.60	126.72	122.80
1	A	915	A	C2-N3-C4	5.60	113.40	110.60
1	A	28	C	C2-N1-C1'	5.59	124.95	118.80
1	A	312	C	C6-N1-C2	-5.59	118.06	120.30
1	A	800	G	C8-N9-C1'	-5.59	119.73	127.00
1	A	1873	U	N1-C2-O2	5.59	126.72	122.80
1	A	1255	C	C6-N1-C2	-5.59	118.06	120.30
1	A	1375	G	C6-N1-C2	-5.59	121.75	125.10
1	A	2329	C	C5-C6-N1	5.59	123.80	121.00
1	A	2455	U	N3-C2-O2	-5.59	118.29	122.20
1	A	2493	U	C5-C6-N1	5.58	125.49	122.70
1	A	2983	C	C6-N1-C1'	-5.58	114.11	120.80
1	A	1298	C	C5-C6-N1	5.57	123.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1156	C	C6-N1-C2	-5.57	118.07	120.30
1	A	2552	C	N3-C2-O2	-5.57	118.00	121.90
1	A	2415	C	C5-C6-N1	5.56	123.78	121.00
1	A	2192	C	C2-N1-C1'	5.56	124.92	118.80
1	A	2382	G	N3-C4-N9	-5.55	122.67	126.00
1	A	618	C	C5-C6-N1	5.55	123.77	121.00
1	A	2274	U	N3-C2-O2	-5.55	118.32	122.20
1	A	1396	C	C6-N1-C2	-5.54	118.08	120.30
1	A	2333	C	N3-C2-O2	-5.54	118.02	121.90
1	A	2842	U	C5-C6-N1	5.54	125.47	122.70
1	A	2422	C	C6-N1-C2	-5.54	118.08	120.30
1	A	2258	U	C2-N1-C1'	5.54	124.34	117.70
1	A	962	A	N7-C8-N9	5.51	116.55	113.80
1	A	1227	C	N3-C2-O2	-5.50	118.05	121.90
1	A	241	G	N7-C8-N9	5.50	115.85	113.10
1	A	2849	C	N3-C2-O2	-5.49	118.06	121.90
1	A	2773	C	C2-N1-C1'	5.49	124.83	118.80
1	A	860	G	C2-N3-C4	5.48	114.64	111.90
1	A	1199	C	C6-N1-C2	5.48	122.49	120.30
1	A	1873	U	N3-C2-O2	-5.48	118.36	122.20
1	A	177	U	N1-C2-O2	5.47	126.63	122.80
1	A	1901	A	C2-N3-C4	5.47	113.34	110.60
1	A	2904	U	N1-C2-O2	5.47	126.63	122.80
1	A	252	U	C6-N1-C2	-5.47	117.72	121.00
1	A	1239	C	C2-N1-C1'	5.46	124.80	118.80
1	A	1878	G	C8-N9-C1'	-5.46	119.91	127.00
1	A	3092	C	C6-N1-C2	-5.46	118.12	120.30
46	x	26	C	C5-C6-N1	5.46	123.73	121.00
1	A	2258	U	C6-N1-C1'	-5.46	113.56	121.20
47	y	113	U	N3-C2-O2	-5.45	118.38	122.20
1	A	2407	C	C2-N3-C4	-5.45	117.17	119.90
1	A	111	C	N1-C2-O2	5.45	122.17	118.90
1	A	2196	C	C2-N1-C1'	5.45	124.79	118.80
1	A	1952	G	C4-N9-C1'	5.45	133.58	126.50
1	A	3306	U	C2-N1-C1'	5.45	124.23	117.70
1	A	3349	C	C6-N1-C2	-5.44	118.12	120.30
47	y	102	U	N1-C2-O2	5.44	126.61	122.80
47	y	64	U	N1-C2-O2	5.44	126.61	122.80
1	A	2331	C	N3-C2-O2	-5.44	118.09	121.90
1	A	2729	U	N1-C2-O2	5.44	126.61	122.80
1	A	104	G	N1-C6-O6	-5.43	116.64	119.90
1	A	1032	C	C6-N1-C2	-5.43	118.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1269	U	C6-N1-C1'	-5.43	113.59	121.20
1	A	1706	C	N1-C2-O2	5.43	122.16	118.90
1	A	2415	C	C6-N1-C2	-5.43	118.13	120.30
1	A	2764	C	N3-C2-O2	-5.43	118.10	121.90
1	A	2508	U	N3-C2-O2	-5.42	118.40	122.20
1	A	960	U	N1-C2-O2	5.42	126.59	122.80
1	A	379	C	N3-C2-O2	-5.42	118.11	121.90
1	A	1943	C	C2-N1-C1'	5.41	124.75	118.80
1	A	2904	U	N3-C2-O2	-5.41	118.41	122.20
1	A	3141	A	C5-C6-N6	-5.41	119.37	123.70
1	A	2951	G	C4-N9-C1'	5.41	133.53	126.50
1	A	82	C	C6-N1-C2	-5.41	118.14	120.30
1	A	179	C	N3-C2-O2	-5.39	118.12	121.90
1	A	1239	C	N3-C2-O2	-5.39	118.12	121.90
47	y	135	G	C8-N9-C1'	5.39	134.01	127.00
1	A	890	C	C6-N1-C2	-5.39	118.14	120.30
1	A	1525	G	C8-N9-C1'	-5.39	119.99	127.00
1	A	2765	C	C6-N1-C2	-5.39	118.14	120.30
1	A	1224	C	C2-N1-C1'	5.38	124.72	118.80
1	A	2690	G	C4-N9-C1'	5.38	133.50	126.50
1	A	507	U	C2-N1-C1'	5.38	124.15	117.70
1	A	982	C	C5-C6-N1	5.38	123.69	121.00
1	A	2566	C	N1-C2-O2	5.38	122.13	118.90
1	A	1052	U	N3-C2-O2	-5.37	118.44	122.20
47	y	85	G	C4-C5-N7	5.37	112.95	110.80
1	A	2265	C	C2-N1-C1'	5.37	124.71	118.80
47	y	113	U	C6-N1-C1'	-5.37	113.69	121.20
1	A	793	C	C6-N1-C2	-5.36	118.16	120.30
1	A	1496	C	C5-C6-N1	5.36	123.68	121.00
1	A	1681	U	N3-C2-O2	-5.35	118.45	122.20
1	A	1827	C	C6-N1-C2	-5.35	118.16	120.30
1	A	2849	C	C2-N1-C1'	5.34	124.68	118.80
1	A	656	A	N7-C8-N9	5.33	116.46	113.80
1	A	1066	G	C4-N9-C1'	5.32	133.42	126.50
1	A	694	C	N3-C2-O2	-5.32	118.18	121.90
1	A	1312	C	N3-C2-O2	-5.32	118.18	121.90
1	A	2490	C	N1-C2-O2	5.32	122.09	118.90
1	A	2824	G	C4-N9-C1'	5.31	133.41	126.50
1	A	1355	A	P-O3'-C3'	5.31	126.07	119.70
1	A	1585	C	C2-N1-C1'	5.31	124.64	118.80
46	x	100	C	N3-C2-O2	-5.31	118.19	121.90
1	A	283	G	C8-N9-C1'	-5.30	120.10	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1614	C	C5-C6-N1	5.30	123.65	121.00
46	x	80	G	C4-C5-N7	5.30	112.92	110.80
1	A	3105	U	C6-N1-C2	-5.30	117.82	121.00
1	A	1255	C	C2-N1-C1'	5.30	124.63	118.80
1	A	1190	A	C4-N9-C1'	5.30	135.83	126.30
1	A	140	C	C6-N1-C2	-5.29	118.18	120.30
1	A	960	U	C6-N1-C1'	-5.29	113.80	121.20
47	y	85	G	C6-C5-N7	-5.29	127.23	130.40
1	A	915	A	C4-N9-C1'	5.29	135.81	126.30
1	A	1287	A	P-O3'-C3'	5.28	126.04	119.70
1	A	1743	G	C8-N9-C1'	-5.28	120.14	127.00
1	A	3161	C	C6-N1-C2	-5.28	118.19	120.30
1	A	3360	C	C5-C6-N1	5.28	123.64	121.00
1	A	2482	U	N1-C2-O2	5.28	126.49	122.80
46	x	105	C	C6-N1-C1'	-5.28	114.47	120.80
1	A	174	C	N3-C2-O2	-5.27	118.21	121.90
1	A	2266	U	N1-C2-O2	5.27	126.49	122.80
1	A	2706	G	C4-N9-C1'	5.27	133.35	126.50
1	A	1896	A	C4-N9-C1'	5.26	135.78	126.30
1	A	2622	C	N3-C2-O2	-5.26	118.21	121.90
1	A	982	C	C6-N1-C2	-5.26	118.19	120.30
1	A	2585	G	C2-N3-C4	5.26	114.53	111.90
1	A	149	U	N1-C2-O2	5.26	126.48	122.80
1	A	916	G	P-O3'-C3'	5.25	126.01	119.70
1	A	1320	C	C5-C6-N1	5.25	123.63	121.00
1	A	1426	C	C6-N1-C2	-5.25	118.20	120.30
1	A	1239	C	C6-N1-C2	-5.25	118.20	120.30
1	A	729	C	C6-N1-C2	-5.25	118.20	120.30
1	A	8	C	C2-N1-C1'	5.25	124.57	118.80
1	A	730	C	C6-N1-C2	-5.24	118.20	120.30
1	A	743	C	C2-N1-C1'	5.23	124.56	118.80
1	A	1159	A	C2-N3-C4	5.23	113.22	110.60
1	A	2824	G	N3-C4-C5	-5.23	125.98	128.60
1	A	818	C	C6-N1-C2	-5.23	118.21	120.30
1	A	1031	C	C6-N1-C1'	-5.23	114.52	120.80
1	A	241	G	C8-N9-C4	-5.23	104.31	106.40
1	A	2181	C	C5-C6-N1	5.22	123.61	121.00
1	A	2879	C	C5-C6-N1	5.22	123.61	121.00
1	A	2996	U	N1-C2-O2	5.22	126.45	122.80
1	A	3161	C	N3-C2-O2	-5.22	118.24	121.90
1	A	958	C	N1-C2-O2	5.22	122.03	118.90
1	A	2407	C	N1-C2-N3	5.21	122.85	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1532	C	C2-N1-C1'	5.21	124.53	118.80
1	A	311	C	N1-C2-O2	5.20	122.02	118.90
1	A	193	C	N1-C2-N3	5.20	122.84	119.20
1	A	3092	C	C5-C6-N1	5.20	123.60	121.00
1	A	2239	G	N1-C6-O6	-5.19	116.79	119.90
1	A	2266	U	C2-N1-C1'	5.19	123.92	117.70
1	A	2622	C	C5-C6-N1	5.19	123.59	121.00
1	A	180	C	C6-N1-C2	-5.18	118.23	120.30
43	o	175	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	2772	C	N1-C2-O2	5.18	122.01	118.90
46	x	58	C	N1-C2-O2	5.18	122.00	118.90
1	A	1482	A	C4-N9-C1'	5.17	135.60	126.30
1	A	2405	C	C5-C6-N1	5.17	123.58	121.00
1	A	863	C	C2-N1-C1'	5.17	124.48	118.80
1	A	2277	C	C6-N1-C2	-5.16	118.23	120.30
1	A	1443	G	C4-N9-C1'	5.16	133.21	126.50
1	A	421	G	C8-N9-C1'	-5.16	120.30	127.00
1	A	861	C	N1-C2-O2	5.16	122.00	118.90
1	A	174	C	N1-C2-O2	5.16	121.99	118.90
1	A	1698	C	C6-N1-C2	-5.16	118.24	120.30
1	A	271	C	C6-N1-C2	-5.15	118.24	120.30
1	A	3132	C	N1-C2-O2	5.14	121.99	118.90
1	A	800	G	N3-C4-C5	-5.14	126.03	128.60
1	A	1276	U	C5-C6-N1	5.14	125.27	122.70
1	A	2418	G	C4-N9-C1'	5.14	133.18	126.50
1	A	2263	C	C6-N1-C1'	-5.14	114.63	120.80
1	A	179	C	C6-N1-C2	-5.14	118.24	120.30
1	A	2899	C	N1-C2-O2	5.14	121.98	118.90
1	A	1269	U	C5-C6-N1	5.14	125.27	122.70
1	A	2550	U	N1-C2-O2	5.14	126.40	122.80
43	o	409	LEU	C-N-CD	-5.13	109.31	120.60
46	x	80	G	C6-C5-N7	-5.13	127.32	130.40
1	A	863	C	C6-N1-C2	-5.13	118.25	120.30
1	A	1018	G	C4-N9-C1'	5.13	133.17	126.50
1	A	2473	C	C6-N1-C2	-5.13	118.25	120.30
1	A	1218	U	N3-C2-O2	-5.12	118.61	122.20
1	A	2418	G	N3-C4-N9	5.12	129.07	126.00
1	A	2207	A	O4'-C1'-N9	5.12	112.30	108.20
47	y	85	G	P-O3'-C3'	5.12	125.84	119.70
1	A	1563	C	C6-N1-C2	-5.11	118.25	120.30
1	A	1115	G	C4-N9-C1'	5.11	133.15	126.50
1	A	2192	C	C6-N1-C2	-5.11	118.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1878	G	N3-C4-C5	-5.11	126.05	128.60
1	A	1309	U	N3-C2-O2	-5.10	118.63	122.20
1	A	1196	C	C6-N1-C2	-5.10	118.26	120.30
1	A	113	C	C6-N1-C2	-5.09	118.26	120.30
1	A	922	U	C6-N1-C2	-5.09	117.95	121.00
1	A	111	C	N3-C2-O2	-5.08	118.34	121.90
1	A	2476	C	C6-N1-C2	-5.08	118.27	120.30
1	A	2904	U	C2-N1-C1'	5.08	123.80	117.70
1	A	311	C	C6-N1-C2	-5.08	118.27	120.30
1	A	2202	C	C6-N1-C2	-5.07	118.27	120.30
1	A	2925	C	C6-N1-C2	-5.07	118.27	120.30
1	A	1353	U	N3-C2-O2	-5.07	118.65	122.20
1	A	601	U	C5-C6-N1	5.07	125.23	122.70
1	A	3360	C	C6-N1-C2	-5.07	118.27	120.30
46	x	80	G	N1-C6-O6	5.07	122.94	119.90
1	A	1597	C	C6-N1-C2	-5.06	118.28	120.30
1	A	1907	C	C6-N1-C1'	-5.06	114.73	120.80
1	A	632	G	C4-N9-C1'	5.06	133.08	126.50
1	A	1681	U	N1-C2-O2	5.06	126.34	122.80
1	A	2824	G	N3-C4-N9	5.06	129.04	126.00
1	A	2943	G	C6-C5-N7	-5.06	127.36	130.40
1	A	1742	U	C5-C6-N1	5.06	125.23	122.70
1	A	140	C	C5-C6-N1	5.05	123.53	121.00
1	A	2879	C	C6-N1-C2	-5.05	118.28	120.30
46	x	100	C	N1-C2-O2	5.05	121.93	118.90
1	A	662	U	C2-N1-C1'	5.05	123.76	117.70
1	A	3166	C	C5-C6-N1	5.05	123.52	121.00
1	A	192	C	N1-C2-O2	5.04	121.92	118.90
1	A	915	A	N3-C4-N9	5.04	131.43	127.40
1	A	2881	C	C6-N1-C2	-5.04	118.28	120.30
1	A	1320	C	C6-N1-C2	-5.04	118.28	120.30
1	A	2551	U	N3-C2-O2	-5.04	118.67	122.20
1	A	1878	G	N3-C4-N9	5.04	129.02	126.00
1	A	2351	U	N3-C2-O2	-5.03	118.68	122.20
1	A	3141	A	N9-C4-C5	-5.03	103.79	105.80
1	A	962	A	C8-N9-C4	-5.03	103.79	105.80
1	A	62	A	N7-C8-N9	5.03	116.31	113.80
1	A	2689	A	C2-N3-C4	5.03	113.11	110.60
1	A	2201	G	C4-N9-C1'	5.03	133.03	126.50
1	A	2274	U	N1-C2-O2	5.03	126.32	122.80
1	A	2617	U	N1-C2-O2	5.03	126.32	122.80
1	A	1708	C	N1-C2-O2	5.02	121.91	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3303	G	OP1-P-O3'	5.02	116.25	105.20
1	A	3078	U	C2-N1-C1'	5.02	123.73	117.70
1	A	753	C	C6-N1-C2	-5.01	118.30	120.30
1	A	1146	C	C6-N1-C2	-5.01	118.30	120.30
1	A	2497	U	C6-N1-C2	-5.01	118.00	121.00
1	A	1710	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	245/254 (96%)	217 (89%)	28 (11%)	0	100	100
3	C	379/387 (98%)	338 (89%)	40 (11%)	1 (0%)	41	75
4	D	359/362 (99%)	331 (92%)	28 (8%)	0	100	100
5	E	167/174 (96%)	153 (92%)	14 (8%)	0	100	100
6	F	187/191 (98%)	177 (95%)	10 (5%)	0	100	100
7	G	173/176 (98%)	153 (88%)	20 (12%)	0	100	100
8	H	221/256 (86%)	207 (94%)	14 (6%)	0	100	100
9	J	195/198 (98%)	187 (96%)	8 (4%)	0	100	100
10	K	184/199 (92%)	165 (90%)	19 (10%)	0	100	100
11	L	134/137 (98%)	124 (92%)	10 (8%)	0	100	100
12	M	133/138 (96%)	125 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	N	146/149 (98%)	124 (85%)	22 (15%)	0	100	100
14	O	201/204 (98%)	188 (94%)	13 (6%)	0	100	100
15	P	267/297 (90%)	251 (94%)	16 (6%)	0	100	100
16	Q	183/186 (98%)	169 (92%)	14 (8%)	0	100	100
17	R	148/189 (78%)	144 (97%)	4 (3%)	0	100	100
18	S	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
19	T	157/160 (98%)	142 (90%)	15 (10%)	0	100	100
20	U	152/184 (83%)	138 (91%)	14 (9%)	0	100	100
21	V	97/121 (80%)	88 (91%)	9 (9%)	0	100	100
22	W	118/142 (83%)	106 (90%)	11 (9%)	1 (1%)	19	57
23	X	123/127 (97%)	114 (93%)	9 (7%)	0	100	100
24	Y	133/136 (98%)	121 (91%)	12 (9%)	0	100	100
25	Z	116/120 (97%)	106 (91%)	10 (9%)	0	100	100
26	a	50/59 (85%)	42 (84%)	8 (16%)	0	100	100
27	b	217/244 (89%)	197 (91%)	20 (9%)	0	100	100
28	c	95/105 (90%)	93 (98%)	2 (2%)	0	100	100
29	d	105/113 (93%)	88 (84%)	17 (16%)	0	100	100
30	e	125/130 (96%)	112 (90%)	12 (10%)	1 (1%)	19	57
31	f	104/107 (97%)	93 (89%)	11 (11%)	0	100	100
32	g	101/121 (84%)	87 (86%)	14 (14%)	0	100	100
33	h	96/100 (96%)	90 (94%)	6 (6%)	0	100	100
34	i	82/88 (93%)	72 (88%)	9 (11%)	1 (1%)	13	49
35	j	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
36	k	48/51 (94%)	40 (83%)	8 (17%)	0	100	100
37	l	92/106 (87%)	84 (91%)	8 (9%)	0	100	100
38	m	87/92 (95%)	77 (88%)	10 (12%)	0	100	100
39	n	222/245 (91%)	195 (88%)	27 (12%)	0	100	100
40	z	56/432 (13%)	47 (84%)	9 (16%)	0	100	100
41	w	387/518 (75%)	347 (90%)	37 (10%)	3 (1%)	19	57
42	v	58/155 (37%)	57 (98%)	1 (2%)	0	100	100
43	o	316/640 (49%)	252 (80%)	58 (18%)	6 (2%)	8	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	s	126/364 (35%)	99 (79%)	24 (19%)	3 (2%)	6	37
All	All	6829/8407 (81%)	6174 (90%)	639 (9%)	16 (0%)	50	79

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	18	PRO
22	W	129	ASP
30	e	7	PRO
41	w	61	CYS
41	w	62	GLU
43	o	174	GLU
43	o	344	TYR
43	o	503	PRO
45	s	323	ARG
43	o	345	PRO
45	s	310	CYS
45	s	311	SER
34	i	37	CYS
41	w	25	PRO
43	o	381	ASP
43	o	428	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	189/196 (96%)	189 (100%)	0	100	100
3	C	317/323 (98%)	311 (98%)	6 (2%)	57	75
4	D	288/289 (100%)	282 (98%)	6 (2%)	53	73
5	E	147/150 (98%)	144 (98%)	3 (2%)	55	74
6	F	169/171 (99%)	169 (100%)	0	100	100
7	G	152/153 (99%)	150 (99%)	2 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	183/208 (88%)	183 (100%)	0	100	100
9	J	163/164 (99%)	162 (99%)	1 (1%)	86	91
10	K	149/159 (94%)	148 (99%)	1 (1%)	84	90
11	L	104/105 (99%)	103 (99%)	1 (1%)	76	86
12	M	107/109 (98%)	106 (99%)	1 (1%)	78	87
13	N	118/119 (99%)	118 (100%)	0	100	100
14	O	175/176 (99%)	175 (100%)	0	100	100
15	P	227/245 (93%)	227 (100%)	0	100	100
16	Q	150/151 (99%)	149 (99%)	1 (1%)	84	90
17	R	124/154 (80%)	124 (100%)	0	100	100
18	S	155/156 (99%)	154 (99%)	1 (1%)	86	91
19	T	136/137 (99%)	133 (98%)	3 (2%)	52	71
20	U	125/146 (86%)	124 (99%)	1 (1%)	81	89
21	V	86/107 (80%)	86 (100%)	0	100	100
22	W	104/118 (88%)	103 (99%)	1 (1%)	76	86
23	X	108/110 (98%)	107 (99%)	1 (1%)	78	87
24	Y	115/116 (99%)	114 (99%)	1 (1%)	78	87
25	Z	104/105 (99%)	103 (99%)	1 (1%)	76	86
26	a	41/47 (87%)	41 (100%)	0	100	100
27	b	184/205 (90%)	183 (100%)	1 (0%)	88	93
28	c	81/88 (92%)	81 (100%)	0	100	100
29	d	94/97 (97%)	94 (100%)	0	100	100
30	e	109/111 (98%)	105 (96%)	4 (4%)	34	60
31	f	90/91 (99%)	90 (100%)	0	100	100
32	g	88/103 (85%)	85 (97%)	3 (3%)	37	62
33	h	80/82 (98%)	79 (99%)	1 (1%)	69	82
34	i	69/71 (97%)	68 (99%)	1 (1%)	67	81
35	j	68/69 (99%)	66 (97%)	2 (3%)	42	65
36	k	45/46 (98%)	43 (96%)	2 (4%)	28	56
37	l	81/91 (89%)	78 (96%)	3 (4%)	34	60
38	m	70/72 (97%)	66 (94%)	4 (6%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	n	192/211 (91%)	189 (98%)	3 (2%)	62	79
40	z	53/392 (14%)	52 (98%)	1 (2%)	57	75
41	w	348/467 (74%)	335 (96%)	13 (4%)	34	60
42	v	53/129 (41%)	49 (92%)	4 (8%)	13	42
43	o	284/555 (51%)	254 (89%)	30 (11%)	6	29
45	s	110/323 (34%)	99 (90%)	11 (10%)	7	30
All	All	5835/7117 (82%)	5721 (98%)	114 (2%)	57	74

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	17	LEU
3	C	18	PRO
3	C	19	ARG
3	C	97	ARG
3	C	244	ARG
3	C	332	ARG
4	D	82	THR
4	D	103	THR
4	D	138	ARG
4	D	148	ILE
4	D	260	GLN
4	D	275	THR
5	E	55	ARG
5	E	92	ARG
5	E	174	LYS
7	G	139	LYS
7	G	152	THR
9	J	61	THR
10	K	104	ARG
11	L	49	LEU
12	M	108	ARG
16	Q	186	VAL
18	S	172	TYR
19	T	83	ARG
19	T	112	ASN
19	T	136	ARG
20	U	138	LYS
22	W	127	THR
23	X	51	ARG

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Mol	Chain	Res	Type
24	Y	60	LYS
25	Z	81	ARG
27	b	244	ASN
30	e	3	SER
30	e	4	LEU
30	e	6	HIS
30	e	8	LYS
32	g	47	CYS
32	g	80	ARG
32	g	81	CYS
33	h	100	HIS
34	i	36	SER
35	j	6	THR
35	j	78	LEU
36	k	23	LEU
36	k	51	ILE
37	l	53	GLN
37	l	54	THR
37	l	77	CYS
38	m	39	CYS
38	m	41	PHE
38	m	42	CYS
38	m	60	CYS
39	n	4	ARG
39	n	86	ASN
39	n	205	VAL
40	z	419	ARG
41	w	34	MET
41	w	63	ARG
41	w	65	LEU
41	w	87	ARG
41	w	115	LYS
41	w	143	CYS
41	w	162	ARG
41	w	220	ILE
41	w	221	LYS
41	w	233	THR
41	w	246	VAL
41	w	248	ILE
41	w	249	VAL
42	v	49	ILE
42	v	52	THR

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Mol	Chain	Res	Type
42	v	53	VAL
42	v	58	HIS
43	o	157	GLU
43	o	159	PHE
43	o	160	LEU
43	o	161	GLU
43	o	163	ARG
43	o	165	LYS
43	o	170	GLN
43	o	171	GLU
43	o	173	ASN
43	o	177	LEU
43	o	178	LEU
43	o	213	PHE
43	o	242	THR
43	o	304	LYS
43	o	344	TYR
43	o	349	LYS
43	o	365	SER
43	o	366	SER
43	o	367	THR
43	o	400	LYS
43	o	402	GLU
43	o	409	LEU
43	o	431	TYR
43	o	488	LEU
43	o	495	LYS
43	o	496	LEU
43	o	497	LEU
43	o	499	VAL
43	o	500	ASN
43	o	503	PRO
45	s	231	ARG
45	s	232	CYS
45	s	233	LYS
45	s	296	GLN
45	s	305	PHE
45	s	306	SER
45	s	307	CYS
45	s	323	ARG
45	s	325	SER
45	s	326	CYS

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Mol	Chain	Res	Type
45	s	328	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
41	w	60	ASN
43	o	170	GLN
45	s	282	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3141/3396 (92%)	811 (25%)	17 (0%)
46	x	120/121 (99%)	29 (24%)	0
47	y	155/158 (98%)	32 (20%)	0
All	All	3416/3675 (92%)	872 (25%)	17 (0%)

All (872) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	G
1	A	6	A
1	A	22	G
1	A	26	A
1	A	38	U
1	A	40	A
1	A	41	G
1	A	43	A
1	A	45	A
1	A	49	A
1	A	57	A
1	A	59	G
1	A	60	A
1	A	65	A
1	A	66	A
1	A	70	A
1	A	72	C
1	A	73	C
1	A	75	G
1	A	89	A

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Mol	Chain	Res	Type
1	A	92	G
1	A	99	A
1	A	109	A
1	A	110	G
1	A	111	C
1	A	113	C
1	A	115	A
1	A	116	A
1	A	117	U
1	A	118	U
1	A	119	U
1	A	120	G
1	A	121	A
1	A	122	A
1	A	133	U
1	A	134	U
1	A	135	C
1	A	136	G
1	A	146	U
1	A	147	U
1	A	154	U
1	A	156	G
1	A	157	A
1	A	163	C
1	A	166	C
1	A	171	G
1	A	176	G
1	A	187	A
1	A	190	U
1	A	191	U
1	A	194	U
1	A	198	A
1	A	199	A
1	A	200	C
1	A	206	G
1	A	211	A
1	A	212	G
1	A	213	A
1	A	218	G
1	A	219	A
1	A	220	G
1	A	234	G

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Mol	Chain	Res	Type
1	A	239	G
1	A	241	G
1	A	246	U
1	A	249	U
1	A	250	U
1	A	251	G
1	A	252	U
1	A	257	U
1	A	258	G
1	A	266	A
1	A	269	G
1	A	270	U
1	A	281	G
1	A	286	U
1	A	295	A
1	A	305	U
1	A	315	C
1	A	323	A
1	A	329	U
1	A	334	A
1	A	343	U
1	A	346	C
1	A	349	A
1	A	351	A
1	A	352	A
1	A	353	G
1	A	375	A
1	A	376	G
1	A	385	A
1	A	387	A
1	A	390	G
1	A	395	A
1	A	398	A
1	A	401	U
1	A	402	A
1	A	403	C
1	A	404	G
1	A	420	G
1	A	421	G
1	A	422	A
1	A	437	G
1	A	438	A

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Mol	Chain	Res	Type
1	A	439	C
1	A	440	A
1	A	503	C
1	A	521	A
1	A	523	A
1	A	536	U
1	A	538	G
1	A	541	U
1	A	542	G
1	A	545	U
1	A	546	C
1	A	547	G
1	A	551	A
1	A	557	A
1	A	558	U
1	A	559	A
1	A	569	A
1	A	578	A
1	A	579	G
1	A	589	A
1	A	592	A
1	A	597	G
1	A	600	G
1	A	609	G
1	A	610	G
1	A	611	A
1	A	620	U
1	A	621	A
1	A	622	A
1	A	623	U
1	A	637	C
1	A	645	A
1	A	649	A
1	A	677	A
1	A	681	U
1	A	683	U
1	A	689	U
1	A	690	A
1	A	691	A
1	A	692	A
1	A	698	U
1	A	699	A

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Mol	Chain	Res	Type
1	A	712	G
1	A	715	A
1	A	716	A
1	A	719	U
1	A	720	A
1	A	742	G
1	A	750	G
1	A	765	C
1	A	767	U
1	A	774	G
1	A	776	U
1	A	777	U
1	A	780	A
1	A	781	G
1	A	784	A
1	A	785	G
1	A	786	A
1	A	801	A
1	A	806	A
1	A	808	A
1	A	817	A
1	A	826	G
1	A	830	A
1	A	831	G
1	A	832	G
1	A	837	A
1	A	838	G
1	A	845	G
1	A	847	A
1	A	848	A
1	A	849	C
1	A	857	G
1	A	861	C
1	A	869	G
1	A	874	U
1	A	879	U
1	A	880	G
1	A	881	C
1	A	884	A
1	A	895	A
1	A	896	A
1	A	907	G

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Mol	Chain	Res	Type
1	A	908	G
1	A	914	A
1	A	916	G
1	A	917	A
1	A	920	A
1	A	923	C
1	A	924	G
1	A	932	U
1	A	933	A
1	A	936	A
1	A	937	G
1	A	938	C
1	A	941	G
1	A	943	U
1	A	944	C
1	A	951	A
1	A	953	G
1	A	954	U
1	A	959	C
1	A	960	U
1	A	962	A
1	A	974	G
1	A	979	U
1	A	980	A
1	A	981	U
1	A	982	C
1	A	984	G
1	A	991	G
1	A	994	G
1	A	1000	C
1	A	1001	G
1	A	1003	A
1	A	1004	U
1	A	1007	U
1	A	1008	U
1	A	1009	A
1	A	1010	G
1	A	1011	A
1	A	1012	G
1	A	1013	G
1	A	1014	U
1	A	1016	C

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Mol	Chain	Res	Type
1	A	1017	C
1	A	1018	G
1	A	1022	U
1	A	1025	A
1	A	1026	A
1	A	1027	A
1	A	1028	U
1	A	1029	G
1	A	1032	C
1	A	1033	U
1	A	1035	G
1	A	1036	A
1	A	1037	C
1	A	1038	C
1	A	1041	U
1	A	1043	C
1	A	1045	C
1	A	1050	U
1	A	1051	U
1	A	1063	G
1	A	1064	A
1	A	1065	A
1	A	1066	G
1	A	1079	A
1	A	1081	U
1	A	1087	G
1	A	1090	G
1	A	1093	A
1	A	1094	U
1	A	1095	U
1	A	1096	U
1	A	1098	A
1	A	1103	A
1	A	1104	G
1	A	1116	G
1	A	1117	G
1	A	1126	G
1	A	1128	U
1	A	1129	A
1	A	1130	A
1	A	1131	G
1	A	1132	C

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Mol	Chain	Res	Type
1	A	1137	C
1	A	1143	A
1	A	1144	U
1	A	1145	G
1	A	1151	U
1	A	1158	A
1	A	1159	A
1	A	1160	C
1	A	1168	U
1	A	1177	G
1	A	1179	A
1	A	1180	A
1	A	1181	U
1	A	1192	C
1	A	1193	A
1	A	1195	A
1	A	1196	C
1	A	1200	A
1	A	1201	C
1	A	1209	G
1	A	1216	C
1	A	1217	A
1	A	1218	U
1	A	1219	C
1	A	1220	U
1	A	1222	G
1	A	1225	A
1	A	1232	C
1	A	1233	G
1	A	1236	G
1	A	1240	A
1	A	1241	U
1	A	1242	G
1	A	1243	G
1	A	1245	A
1	A	1246	G
1	A	1247	U
1	A	1248	C
1	A	1249	G
1	A	1253	U
1	A	1258	U
1	A	1262	G

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Mol	Chain	Res	Type
1	A	1263	A
1	A	1265	U
1	A	1266	G
1	A	1269	U
1	A	1270	A
1	A	1271	A
1	A	1272	C
1	A	1273	A
1	A	1274	A
1	A	1277	C
1	A	1278	A
1	A	1279	C
1	A	1280	C
1	A	1285	G
1	A	1288	U
1	A	1289	G
1	A	1295	G
1	A	1301	A
1	A	1302	A
1	A	1307	G
1	A	1309	U
1	A	1313	G
1	A	1317	A
1	A	1325	U
1	A	1330	A
1	A	1332	A
1	A	1348	U
1	A	1349	G
1	A	1350	A
1	A	1351	U
1	A	1352	A
1	A	1353	U
1	A	1354	G
1	A	1355	A
1	A	1356	U
1	A	1357	G
1	A	1362	G
1	A	1386	A
1	A	1394	A
1	A	1399	A
1	A	1400	G
1	A	1417	G

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Mol	Chain	Res	Type
1	A	1418	A
1	A	1419	A
1	A	1421	G
1	A	1434	G
1	A	1435	A
1	A	1436	U
1	A	1437	C
1	A	1446	A
1	A	1450	G
1	A	1455	U
1	A	1465	A
1	A	1475	A
1	A	1478	C
1	A	1481	A
1	A	1482	A
1	A	1488	G
1	A	1496	C
1	A	1508	C
1	A	1512	U
1	A	1523	U
1	A	1527	C
1	A	1539	A
1	A	1542	G
1	A	1544	G
1	A	1555	U
1	A	1556	C
1	A	1560	G
1	A	1562	C
1	A	1563	C
1	A	1566	A
1	A	1567	U
1	A	1568	U
1	A	1570	U
1	A	1571	A
1	A	1572	U
1	A	1573	G
1	A	1574	C
1	A	1576	G
1	A	1577	G
1	A	1580	A
1	A	1581	C
1	A	1583	A

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Mol	Chain	Res	Type
1	A	1589	A
1	A	1593	A
1	A	1605	A
1	A	1606	U
1	A	1618	G
1	A	1619	A
1	A	1620	U
1	A	1629	U
1	A	1631	C
1	A	1636	U
1	A	1642	A
1	A	1643	A
1	A	1657	C
1	A	1675	G
1	A	1677	G
1	A	1681	U
1	A	1683	A
1	A	1713	G
1	A	1715	A
1	A	1724	U
1	A	1725	C
1	A	1741	A
1	A	1750	A
1	A	1751	G
1	A	1753	G
1	A	1760	A
1	A	1762	C
1	A	1763	U
1	A	1764	U
1	A	1765	U
1	A	1766	G
1	A	1794	G
1	A	1797	A
1	A	1808	G
1	A	1809	A
1	A	1813	A
1	A	1814	A
1	A	1816	A
1	A	1820	U
1	A	1821	U
1	A	1835	A
1	A	1839	A

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Mol	Chain	Res	Type
1	A	1841	A
1	A	1842	A
1	A	1846	C
1	A	1847	A
1	A	1849	C
1	A	1850	A
1	A	1866	C
1	A	1878	G
1	A	1880	U
1	A	1886	A
1	A	1893	A
1	A	1901	A
1	A	1906	G
1	A	1907	C
1	A	1913	A
1	A	1920	U
1	A	1926	C
1	A	1930	A
1	A	1931	U
1	A	1948	G
1	A	1952	G
1	A	1953	G
1	A	1954	G
1	A	2095	G
1	A	2100	A
1	A	2101	C
1	A	2102	U
1	A	2107	A
1	A	2112	U
1	A	2113	A
1	A	2114	C
1	A	2117	A
1	A	2121	G
1	A	2122	G
1	A	2125	A
1	A	2131	A
1	A	2139	A
1	A	2140	U
1	A	2145	A
1	A	2149	A
1	A	2158	A
1	A	2159	U

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Mol	Chain	Res	Type
1	A	2160	G
1	A	2169	G
1	A	2171	G
1	A	2176	U
1	A	2185	G
1	A	2187	G
1	A	2188	A
1	A	2192	C
1	A	2196	C
1	A	2201	G
1	A	2205	U
1	A	2206	G
1	A	2209	U
1	A	2244	A
1	A	2249	G
1	A	2253	G
1	A	2256	A
1	A	2257	C
1	A	2258	U
1	A	2261	G
1	A	2262	A
1	A	2263	C
1	A	2264	U
1	A	2265	C
1	A	2266	U
1	A	2268	U
1	A	2269	U
1	A	2270	A
1	A	2273	G
1	A	2274	U
1	A	2279	A
1	A	2281	A
1	A	2282	U
1	A	2286	U
1	A	2287	C
1	A	2294	U
1	A	2295	A
1	A	2298	U
1	A	2306	C
1	A	2307	G
1	A	2308	C
1	A	2310	U

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Mol	Chain	Res	Type
1	A	2313	A
1	A	2314	U
1	A	2315	G
1	A	2334	U
1	A	2336	U
1	A	2356	A
1	A	2361	A
1	A	2364	G
1	A	2365	C
1	A	2366	C
1	A	2372	A
1	A	2373	A
1	A	2374	C
1	A	2375	G
1	A	2380	U
1	A	2388	U
1	A	2393	G
1	A	2394	G
1	A	2397	A
1	A	2398	A
1	A	2400	G
1	A	2401	A
1	A	2402	A
1	A	2403	G
1	A	2404	A
1	A	2405	C
1	A	2411	U
1	A	2412	G
1	A	2417	U
1	A	2422	C
1	A	2434	U
1	A	2435	G
1	A	2437	G
1	A	2439	A
1	A	2444	C
1	A	2446	U
1	A	2449	A
1	A	2453	U
1	A	2454	G
1	A	2455	U
1	A	2456	A
1	A	2457	G

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Mol	Chain	Res	Type
1	A	2458	A
1	A	2459	A
1	A	2460	U
1	A	2461	A
1	A	2462	A
1	A	2464	U
1	A	2465	G
1	A	2466	G
1	A	2467	G
1	A	2468	A
1	A	2470	C
1	A	2471	U
1	A	2472	U
1	A	2474	G
1	A	2475	G
1	A	2479	C
1	A	2481	G
1	A	2483	G
1	A	2484	A
1	A	2485	A
1	A	2487	U
1	A	2489	C
1	A	2490	C
1	A	2492	C
1	A	2493	U
1	A	2494	A
1	A	2495	C
1	A	2496	C
1	A	2498	U
1	A	2501	U
1	A	2502	A
1	A	2503	G
1	A	2505	U
1	A	2506	U
1	A	2511	A
1	A	2514	U
1	A	2515	A
1	A	2527	G
1	A	2549	G
1	A	2550	U
1	A	2551	U
1	A	2553	U

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Mol	Chain	Res	Type
1	A	2555	G
1	A	2558	U
1	A	2561	A
1	A	2568	C
1	A	2569	A
1	A	2570	U
1	A	2571	U
1	A	2572	C
1	A	2573	G
1	A	2585	G
1	A	2586	G
1	A	2593	A
1	A	2594	C
1	A	2606	G
1	A	2607	G
1	A	2614	G
1	A	2617	U
1	A	2618	G
1	A	2619	G
1	A	2626	A
1	A	2629	U
1	A	2635	A
1	A	2652	U
1	A	2656	A
1	A	2657	A
1	A	2672	G
1	A	2674	A
1	A	2677	G
1	A	2679	A
1	A	2680	A
1	A	2688	U
1	A	2689	A
1	A	2691	A
1	A	2694	A
1	A	2703	A
1	A	2704	A
1	A	2705	A
1	A	2708	C
1	A	2713	U
1	A	2714	G
1	A	2716	U
1	A	2719	U

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Mol	Chain	Res	Type
1	A	2720	G
1	A	2728	G
1	A	2729	U
1	A	2734	A
1	A	2740	A
1	A	2746	A
1	A	2749	G
1	A	2753	G
1	A	2755	C
1	A	2762	A
1	A	2771	U
1	A	2772	C
1	A	2777	G
1	A	2778	G
1	A	2796	G
1	A	2797	C
1	A	2799	A
1	A	2800	G
1	A	2801	A
1	A	2802	A
1	A	2803	A
1	A	2810	C
1	A	2814	G
1	A	2817	A
1	A	2822	U
1	A	2824	G
1	A	2828	G
1	A	2832	C
1	A	2834	G
1	A	2836	C
1	A	2842	U
1	A	2843	U
1	A	2844	C
1	A	2845	A
1	A	2846	U
1	A	2847	A
1	A	2849	C
1	A	2850	G
1	A	2851	A
1	A	2856	G
1	A	2859	U
1	A	2869	U

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Mol	Chain	Res	Type
1	A	2871	G
1	A	2872	A
1	A	2873	U
1	A	2875	U
1	A	2887	A
1	A	2888	U
1	A	2889	C
1	A	2897	A
1	A	2898	G
1	A	2899	C
1	A	2900	A
1	A	2907	G
1	A	2935	U
1	A	2936	A
1	A	2938	G
1	A	2941	A
1	A	2947	G
1	A	2955	U
1	A	2971	A
1	A	2976	A
1	A	2977	G
1	A	2978	U
1	A	2983	C
1	A	2997	G
1	A	3011	A
1	A	3012	A
1	A	3021	A
1	A	3022	G
1	A	3027	A
1	A	3030	G
1	A	3039	C
1	A	3056	U
1	A	3059	G
1	A	3078	U
1	A	3079	U
1	A	3080	G
1	A	3091	A
1	A	3092	C
1	A	3094	A
1	A	3101	G
1	A	3104	U
1	A	3113	A

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Mol	Chain	Res	Type
1	A	3116	G
1	A	3118	C
1	A	3119	U
1	A	3122	A
1	A	3130	A
1	A	3131	U
1	A	3141	A
1	A	3142	A
1	A	3153	U
1	A	3154	C
1	A	3155	U
1	A	3156	U
1	A	3157	U
1	A	3158	G
1	A	3164	C
1	A	3165	A
1	A	3170	A
1	A	3171	U
1	A	3173	G
1	A	3175	U
1	A	3176	G
1	A	3179	U
1	A	3181	C
1	A	3186	A
1	A	3187	A
1	A	3197	G
1	A	3206	C
1	A	3207	U
1	A	3210	A
1	A	3213	A
1	A	3216	G
1	A	3217	C
1	A	3218	A
1	A	3219	G
1	A	3221	C
1	A	3268	A
1	A	3270	U
1	A	3271	G
1	A	3273	A
1	A	3275	U
1	A	3276	G
1	A	3279	A

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Mol	Chain	Res	Type
1	A	3280	U
1	A	3281	U
1	A	3282	U
1	A	3289	G
1	A	3293	U
1	A	3294	A
1	A	3295	A
1	A	3304	U
1	A	3313	U
1	A	3316	A
1	A	3317	U
1	A	3320	A
1	A	3323	A
1	A	3332	U
1	A	3335	A
1	A	3340	G
1	A	3341	U
1	A	3342	A
1	A	3345	G
1	A	3346	U
1	A	3349	C
1	A	3351	U
1	A	3352	U
1	A	3353	G
1	A	3354	U
1	A	3356	G
1	A	3367	C
1	A	3369	G
1	A	3378	C
1	A	3381	U
1	A	3382	U
1	A	3386	G
1	A	3389	U
1	A	3393	U
1	A	3396	U
46	x	7	G
46	x	10	C
46	x	11	A
46	x	17	A
46	x	21	G
46	x	22	A
46	x	30	G

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Mol	Chain	Res	Type
46	x	41	G
46	x	42	A
46	x	53	U
46	x	54	U
46	x	55	A
46	x	61	G
46	x	62	U
46	x	63	A
46	x	64	A
46	x	65	G
46	x	67	G
46	x	72	A
46	x	73	C
46	x	76	A
46	x	80	G
46	x	90	U
46	x	91	G
46	x	93	C
46	x	99	G
46	x	102	A
46	x	112	G
46	x	121	U
47	y	23	U
47	y	34	U
47	y	35	C
47	y	37	A
47	y	39	G
47	y	49	G
47	y	50	C
47	y	52	A
47	y	59	A
47	y	62	C
47	y	63	G
47	y	75	G
47	y	80	A
47	y	82	U
47	y	83	C
47	y	84	C
47	y	86	U
47	y	87	G
47	y	90	U
47	y	95	G

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Mol	Chain	Res	Type
47	y	102	U
47	y	103	G
47	y	104	A
47	y	106	C
47	y	109	A
47	y	113	U
47	y	121	U
47	y	125	U
47	y	127	U
47	y	148	G
47	y	151	C
47	y	152	G

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	916	G
1	A	979	U
1	A	1010	G
1	A	1064	A
1	A	1217	A
1	A	1287	A
1	A	1288	U
1	A	1355	A
1	A	1815	U
1	A	2101	C
1	A	2112	U
1	A	2400	G
1	A	2401	A
1	A	2404	A
1	A	3121	U
1	A	3206	C
1	A	3303	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

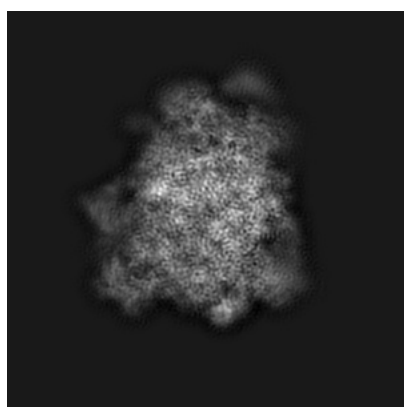
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10071. These allow visual inspection of the internal detail of the map and identification of artifacts.

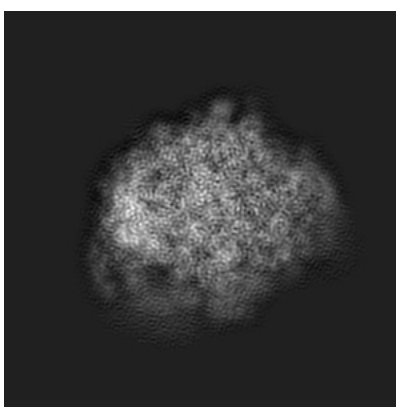
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

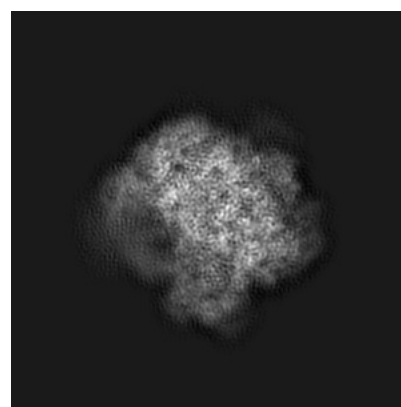
6.1.1 Primary map



X



Y

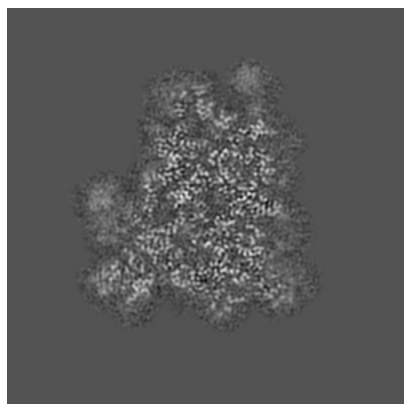


Z

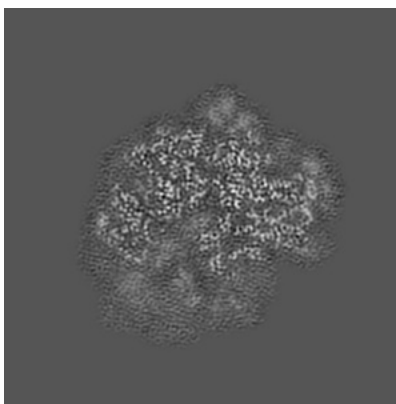
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

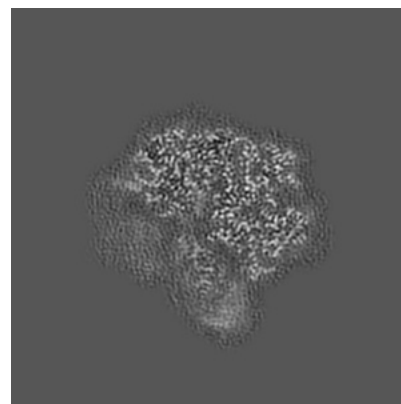
6.2.1 Primary map



X Index: 180



Y Index: 180

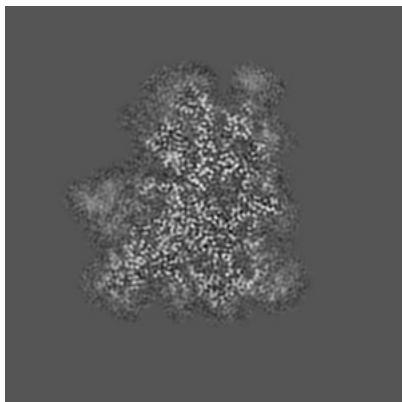


Z Index: 180

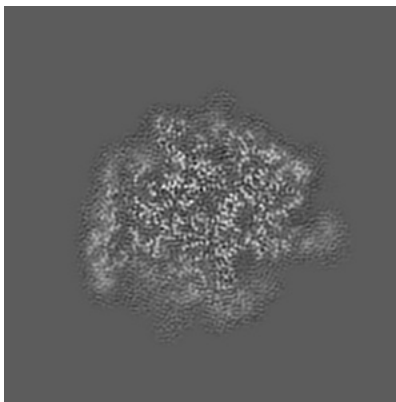
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

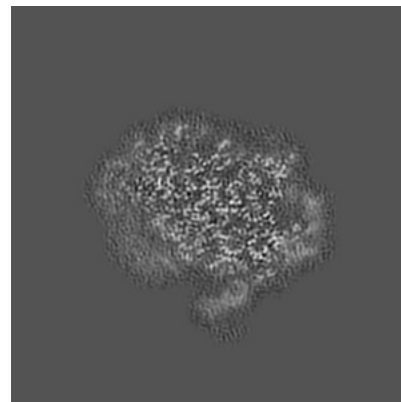
6.3.1 Primary map



X Index: 190



Y Index: 196

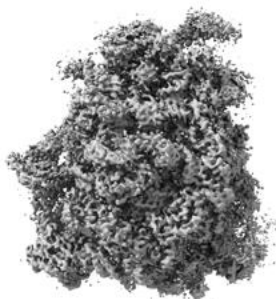


Z Index: 199

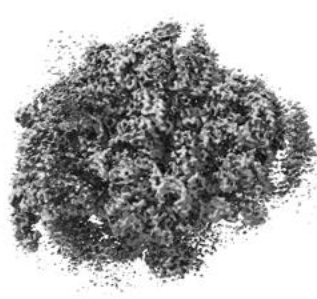
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

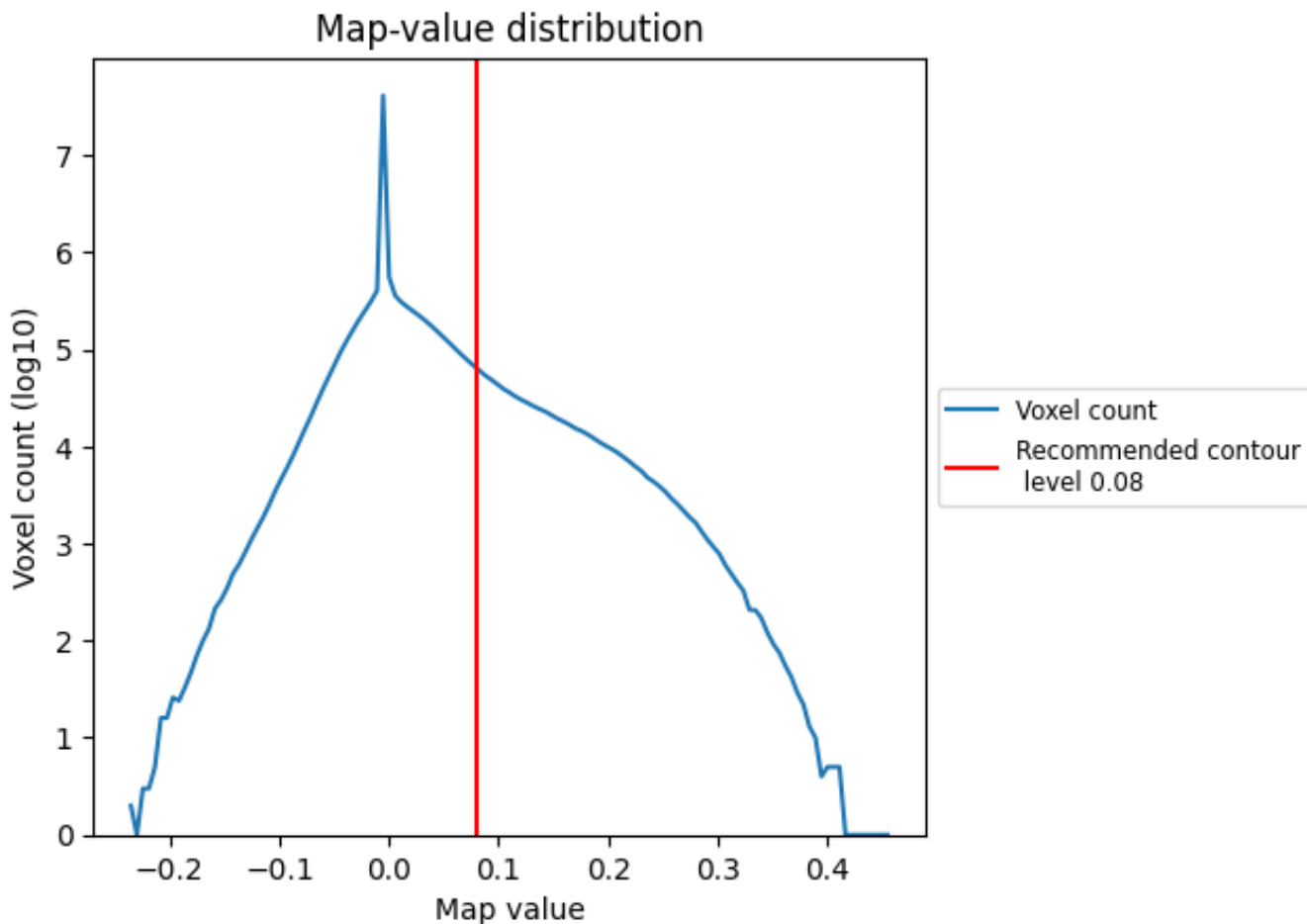
6.5 Mask visualisation

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

7 Map analysis [i](#)

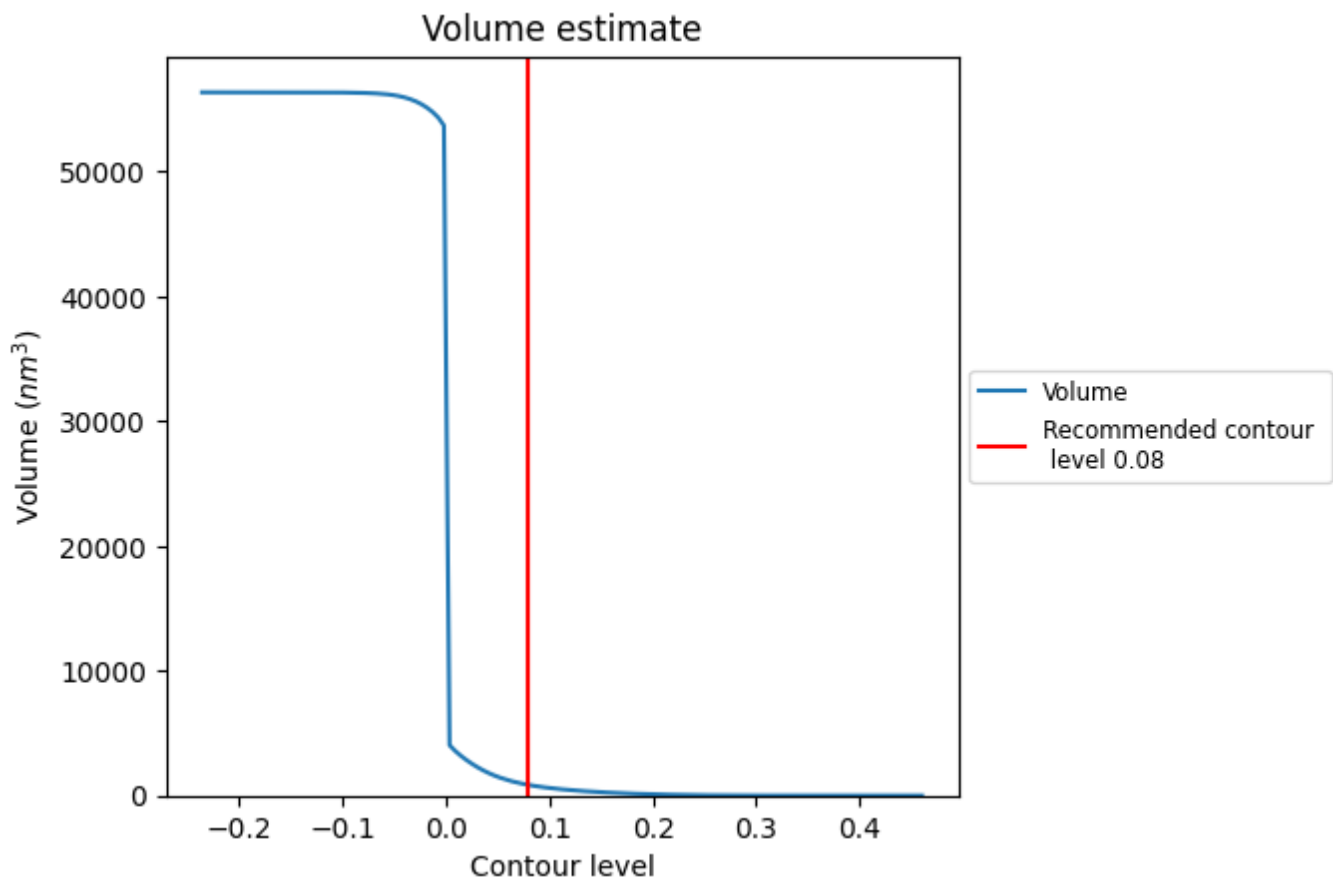
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

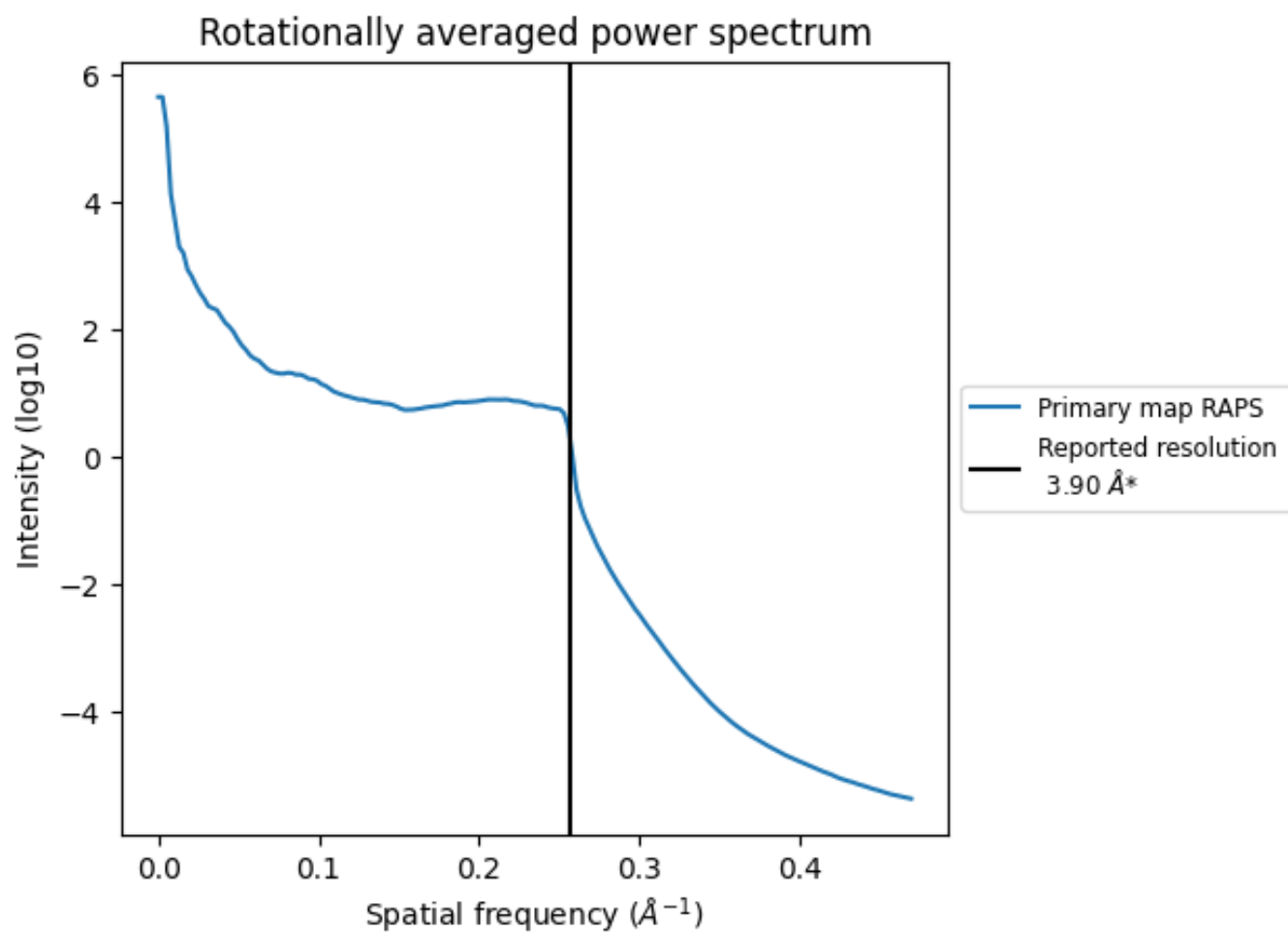
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 854 nm³; this corresponds to an approximate mass of 771 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.256\AA^{-1}

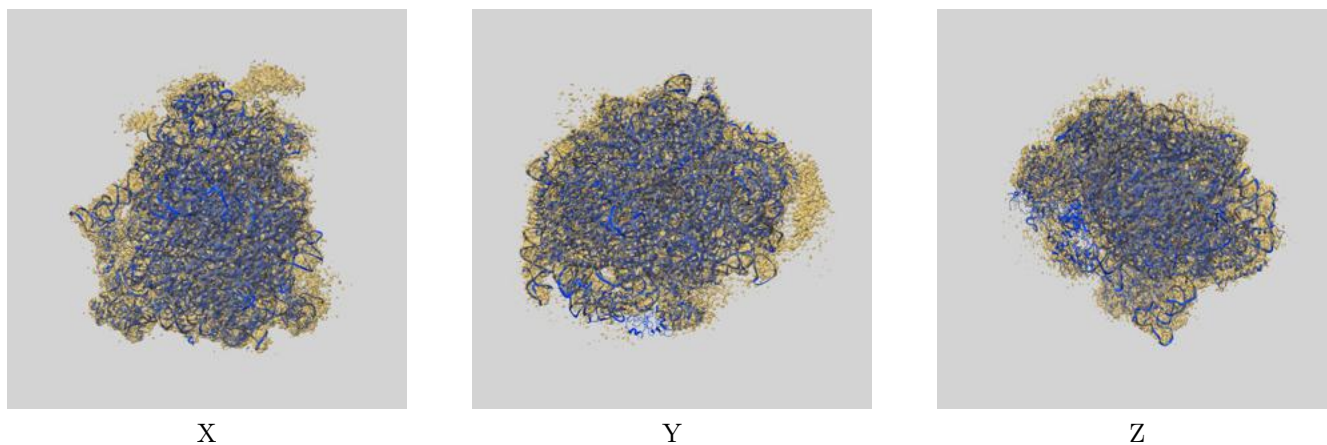
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

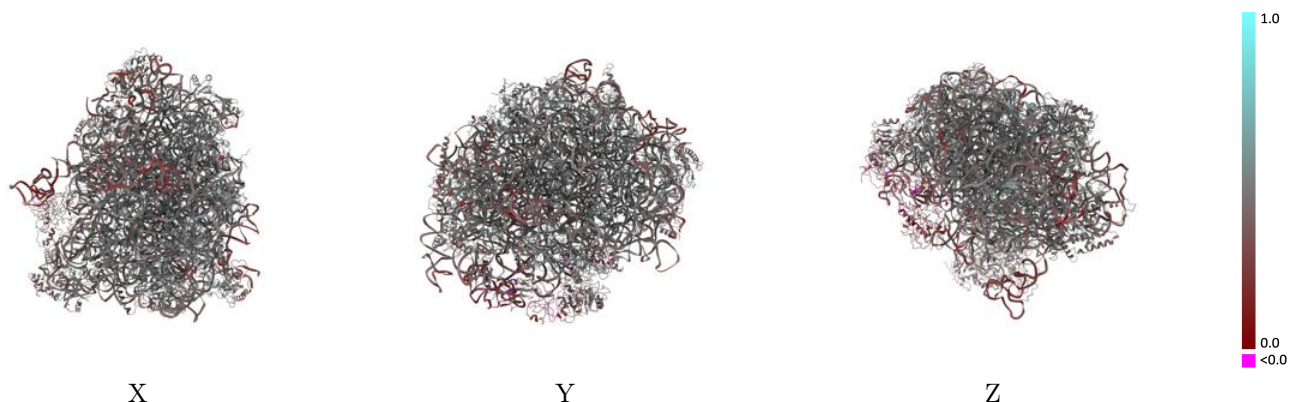
This section contains information regarding the fit between EMDB map EMD-10071 and PDB model 6S05. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



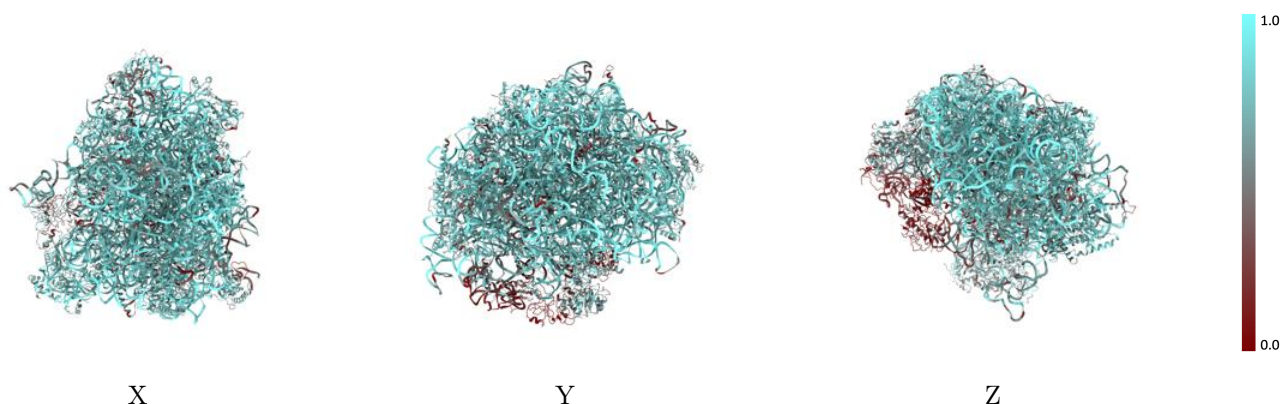
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



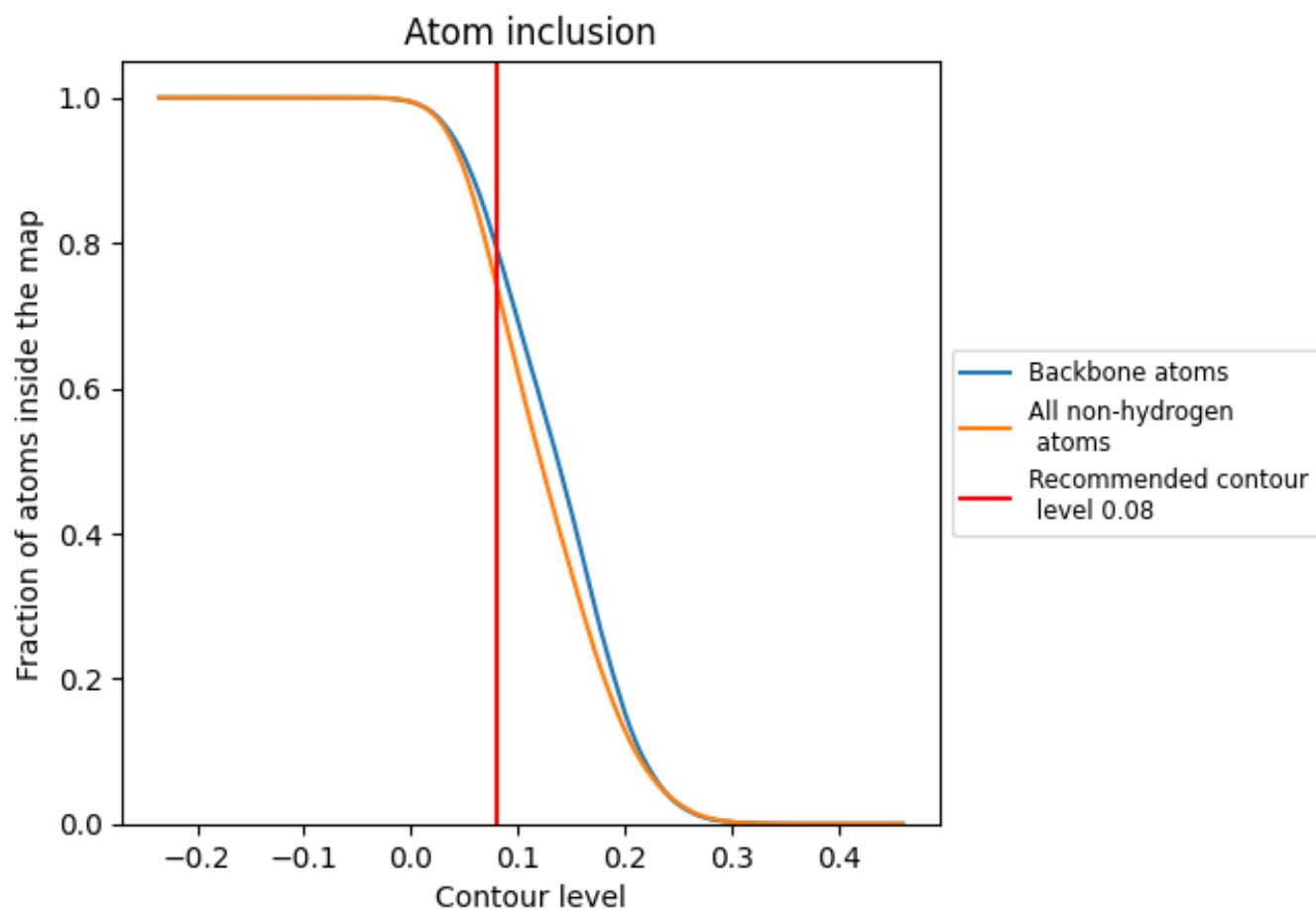
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 74% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7418	 0.4320
A	 0.8033	 0.4180
B	 0.7558	 0.4960
C	 0.7698	 0.4860
D	 0.7755	 0.4980
E	 0.6164	 0.3770
F	 0.4654	 0.3880
G	 0.5863	 0.4140
H	 0.6893	 0.4450
J	 0.7257	 0.4850
K	 0.7291	 0.4740
L	 0.6769	 0.4880
M	 0.7122	 0.4610
N	 0.7765	 0.4970
O	 0.7806	 0.5080
P	 0.7293	 0.4370
Q	 0.7862	 0.5120
R	 0.7739	 0.4820
S	 0.7251	 0.4790
T	 0.7191	 0.4770
U	 0.8035	 0.5060
V	 0.6852	 0.4450
W	 0.7265	 0.4830
X	 0.7879	 0.4920
Y	 0.6832	 0.4340
Z	 0.7876	 0.4830
a	 0.6716	 0.4740
b	 0.7712	 0.4730
c	 0.6722	 0.4210
d	 0.7329	 0.4880
e	 0.7515	 0.5050
f	 0.7610	 0.4960
g	 0.7462	 0.4890
h	 0.5780	 0.4430
i	 0.8109	 0.5150



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Chain	Atom inclusion	Q-score
j	 0.6538	 0.4560
k	 0.7488	 0.5190
l	 0.7371	 0.4990
m	 0.7195	 0.4840
n	 0.5692	 0.4060
o	 0.1273	 0.2660
p	 0.4743	 0.3440
s	 0.0153	 0.1980
v	 0.5289	 0.4540
w	 0.3743	 0.3650
x	 0.9092	 0.4310
y	 0.8961	 0.4560
z	 0.2579	 0.4300