



Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 10:56 pm GMT

PDB ID : 6RBE
EMDB ID : EMD-4793
Title : State 2 of yeast Tsr1-TAP Rps20-Deltaloop pre-40S particles
Authors : Shayan, R.; Mitterer, V.; Ferreira-Cerca, S.; Murat, G.; Enne, T.; Rinaldi, D.; Weigl, S.; Omanic, H.; Gleizes, P.E.; Kressler, D.; Pertschy, B.; Plisson-Chastang, C.
Deposited on : 2019-04-10
Resolution : 3.80 Å (reported)
Based on initial models : ?, 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:

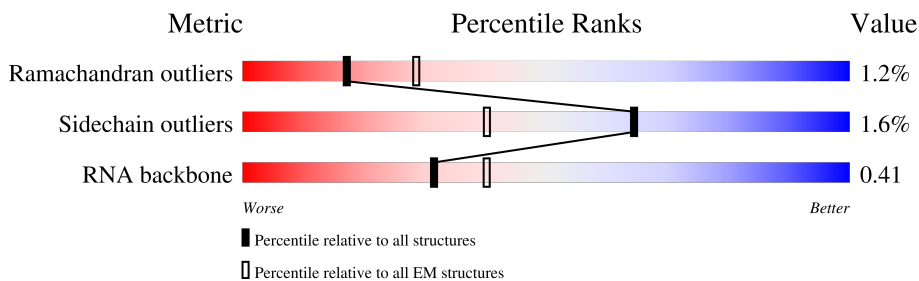
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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	2	1800	
2	A	252	
3	B	255	
4	C	254	
5	E	261	
6	G	236	
7	H	190	
8	I	200	

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Mol	Chain	Length	Quality of chain
9	J	197	88% 5% • 6%
10	L	156	98% ..
11	N	151	94% • • •
12	O	137	87% •
13	R	136	85% • 12%
14	V	87	94% 5% •
15	W	130	96% • •
16	X	145	97% • • •
17	Y	135	94% 5% •
18	b	82	98% • •
19	d	56	88% 7% 5%
20	e	63	90% 5% 5%
21	D	240	88% • 7%
22	F	225	84% 7% 8%
23	K	105	87% • • 9%
24	M	143	75% 11% • 13%
25	P	142	84% • 13%
26	Q	143	93% 5% • •
27	S	146	95% • • •
28	T	144	94% 6% •
29	U	121	79% • 19%
30	Z	108	57% 7% 35%
31	c	67	94% 6%
32	f	152	66% •
33	g	319	98% •

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 72721 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1750	37285	16669	6597	12269	1750	0	0

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	206	1577	1014	278	283	2	0	0

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	113	918	584	169	164	1	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	217	1635	1047	289	297	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	260	2068	1316	389	360	3	0	0

- Molecule 6 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 7 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	H	184	1481	951	265	265	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 9 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	185	1494	943	289	261	1	0	0

- Molecule 10 is a protein called 40S ribosomal protein S11-A.

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

- Molecule 11 is a protein called 40S ribosomal protein S13.

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

- Molecule 12 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	O	18	141	83	35	23	0	0

- Molecule 13 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	R	120	926	577	177	170	2	0	0

- Molecule 14 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 15 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 16 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 17 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 18 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 19 is a protein called 40S ribosomal protein S29-A.

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

- Molecule 20 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	e	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 21 is a protein called 40S ribosomal protein S3.

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

- Molecule 22 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	F	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 23 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	K	96	Total	C	N	O	S	0	0
			772	499	126	145	2		

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 25 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	P	124	Total	C	N	O	S	0	0
			977	622	182	166	7		

- Molecule 26 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 27 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 28 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 29 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	U	98	792	502	144	145	1	0	0

- Molecule 30 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 31 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S31.

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

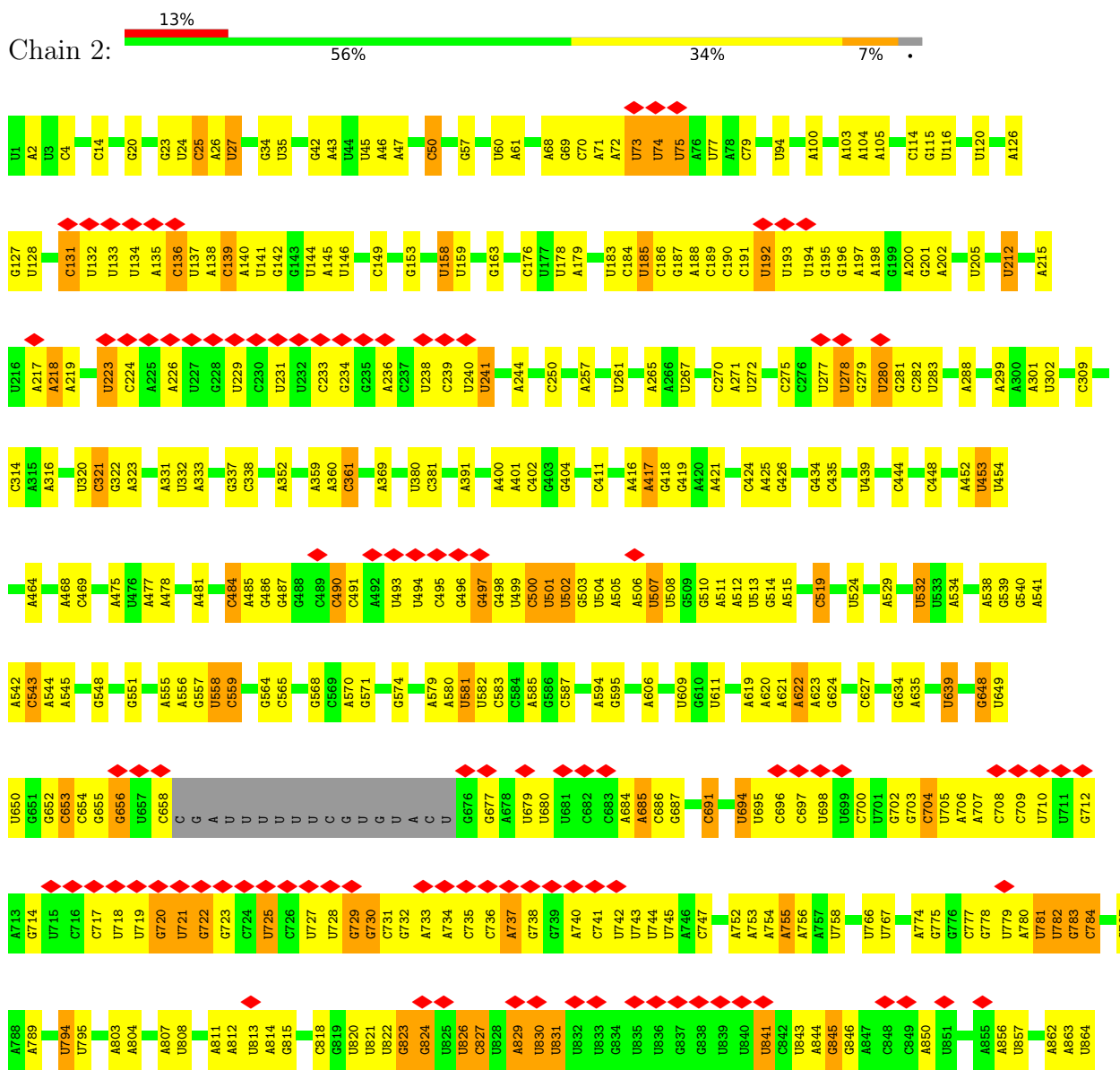
- Molecule 33 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

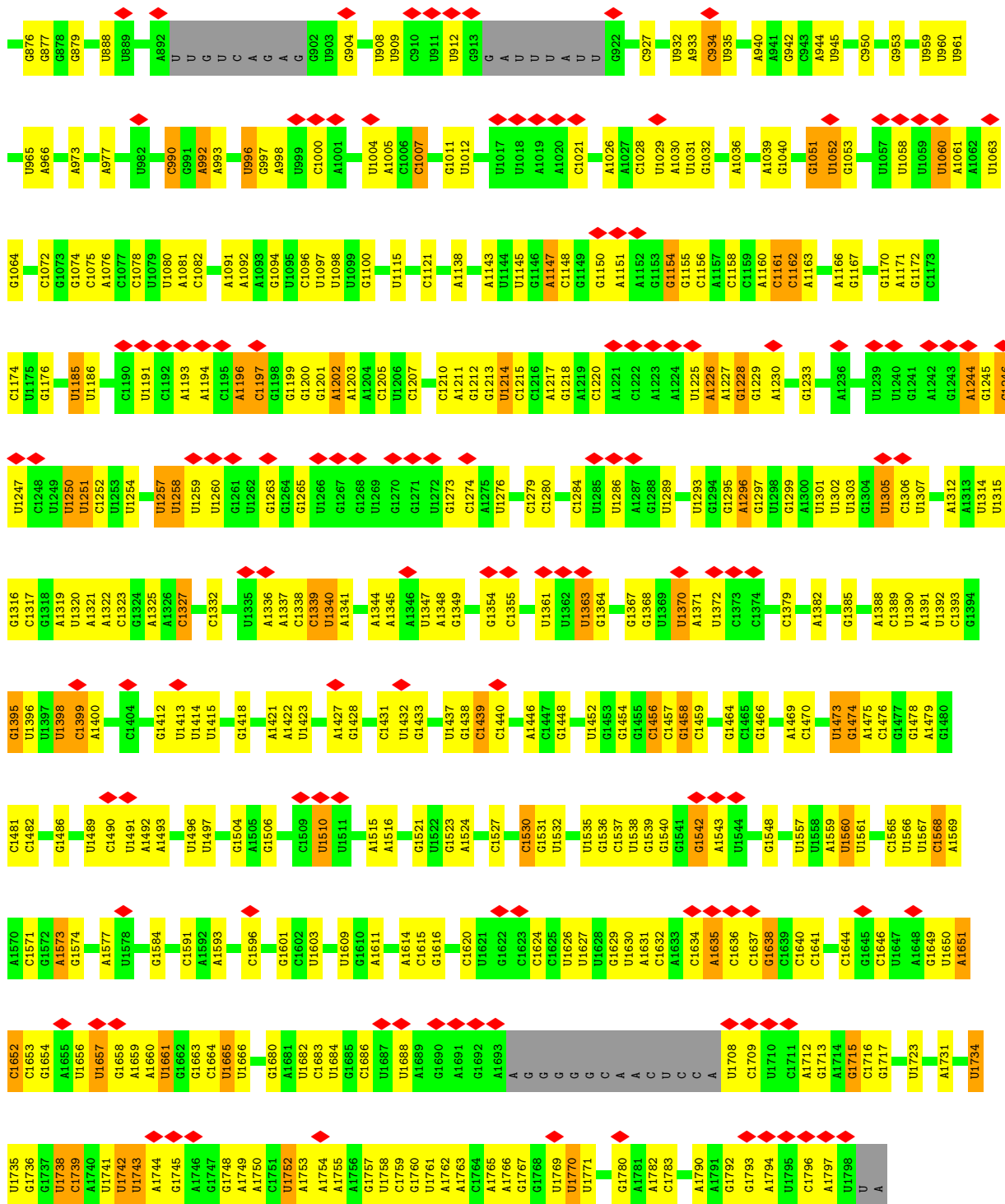
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	g	318	2437	1541	418	470	8	0	0

3 Residue-property plots [i](#)

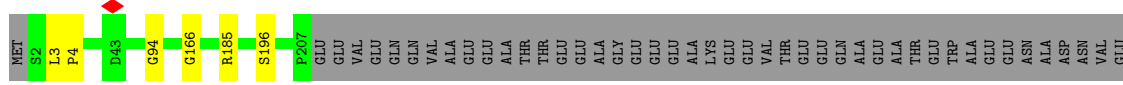
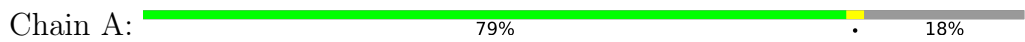
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 18S ribosomal RNA



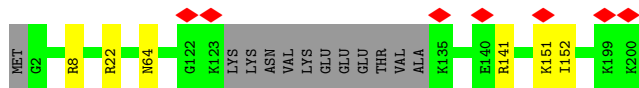
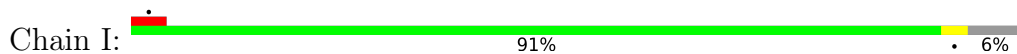


• Molecule 2: 40S ribosomal protein S0-A

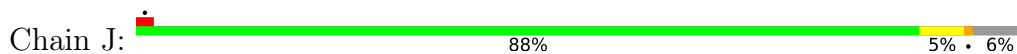




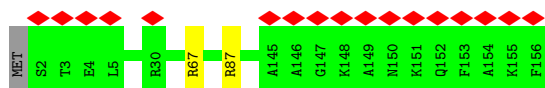
- Molecule 8: 40S ribosomal protein S8-A



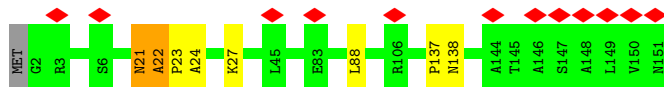
- Molecule 9: 40S ribosomal protein S9-A



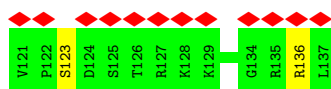
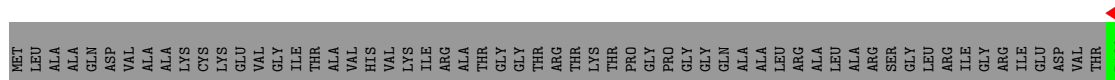
- Molecule 10: 40S ribosomal protein S11-A



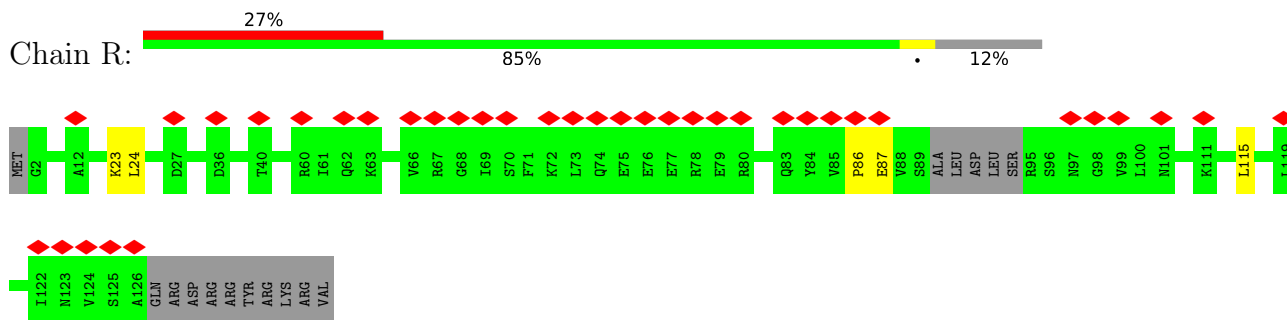
- Molecule 11: 40S ribosomal protein S13



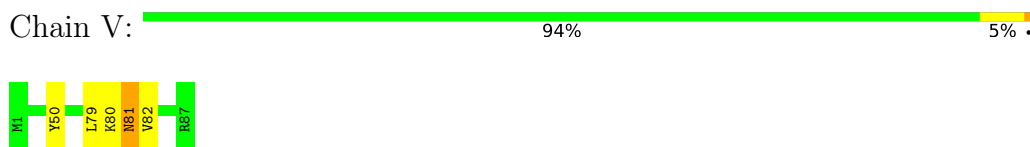
- Molecule 12: 40S ribosomal protein S14-A



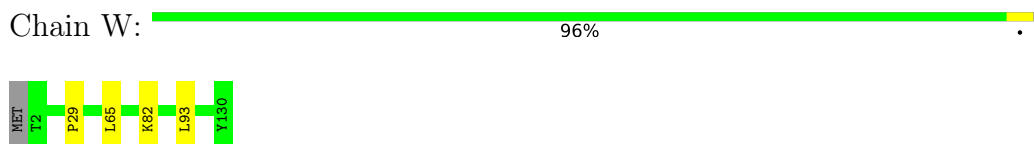
- Molecule 13: 40S ribosomal protein S17-A



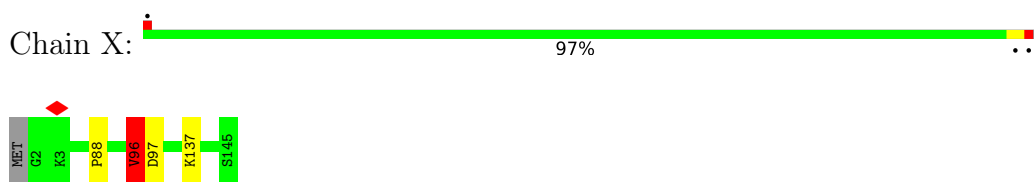
- Molecule 14: 40S ribosomal protein S21-A



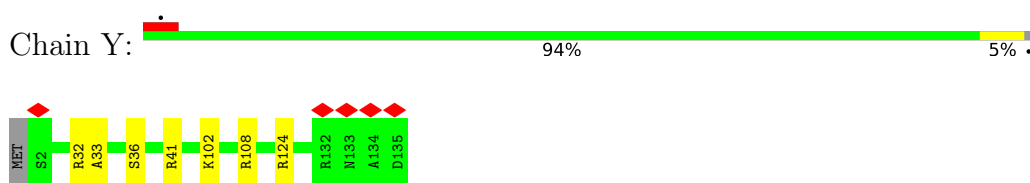
- Molecule 15: 40S ribosomal protein S22-A



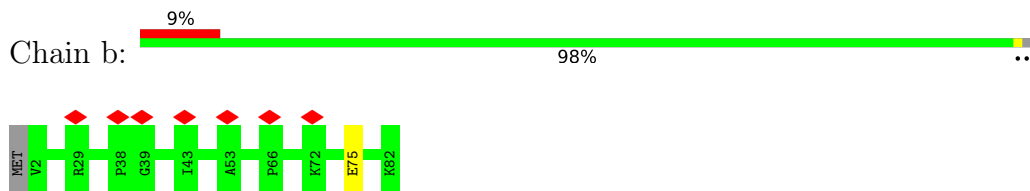
- Molecule 16: 40S ribosomal protein S23-A



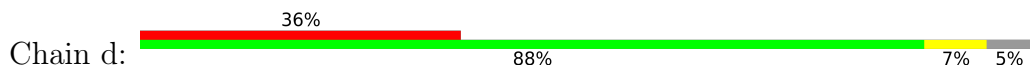
- Molecule 17: 40S ribosomal protein S24-A



- Molecule 18: 40S ribosomal protein S27-A

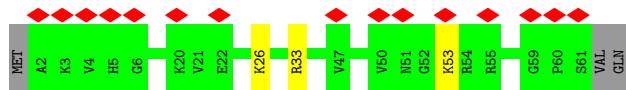
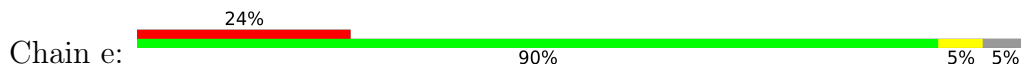


- Molecule 19: 40S ribosomal protein S29-A

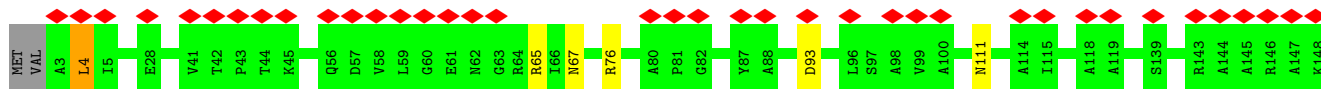
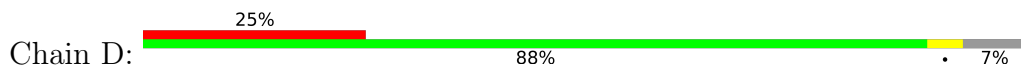




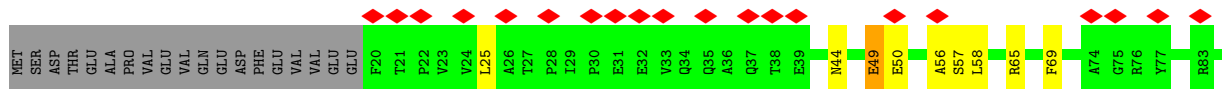
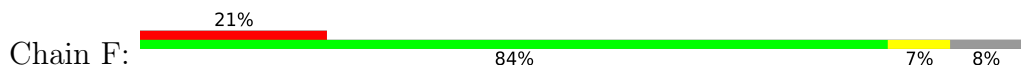
• Molecule 20: 40S ribosomal protein S30-A



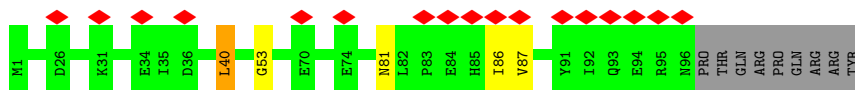
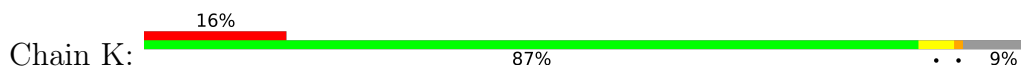
• Molecule 21: 40S ribosomal protein S3



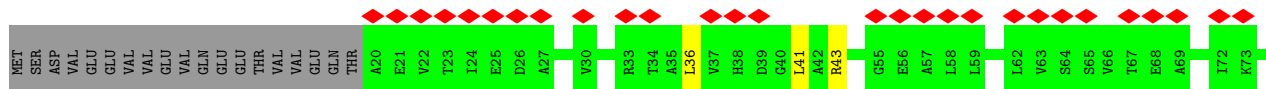
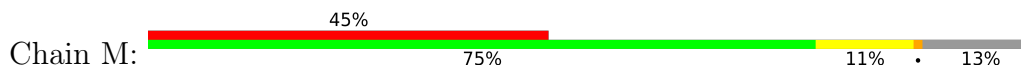
• Molecule 22: 40S ribosomal protein S5

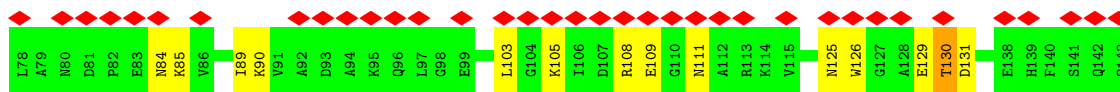


• Molecule 23: 40S ribosomal protein S10-A

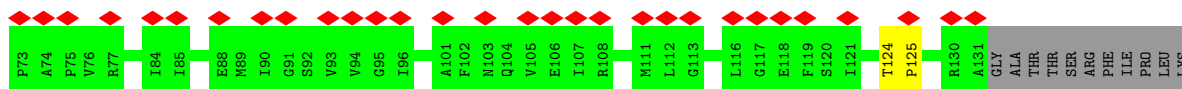
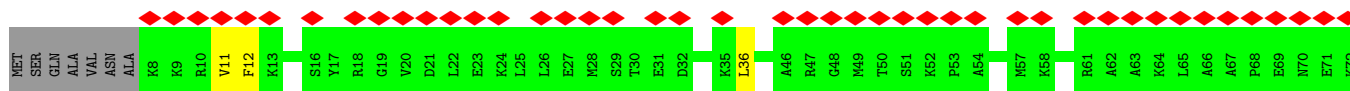
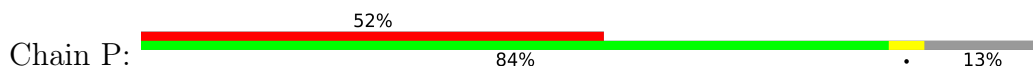


• Molecule 24: 40S ribosomal protein S12

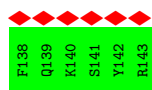
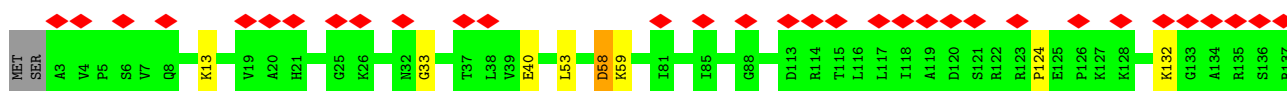
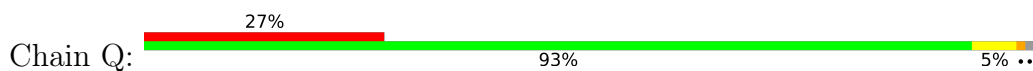




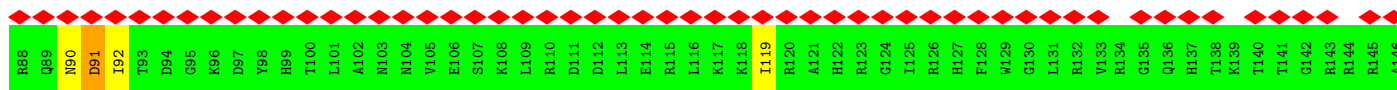
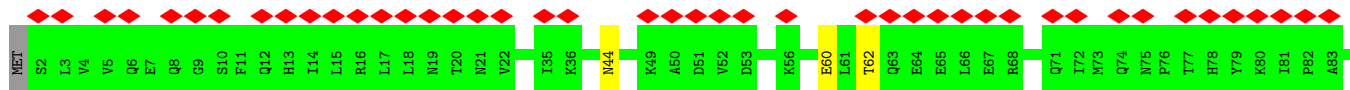
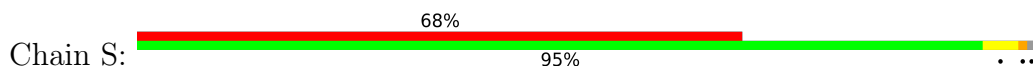
• Molecule 25: 40S ribosomal protein S15



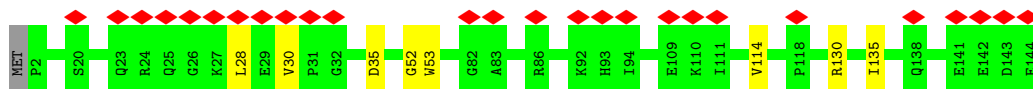
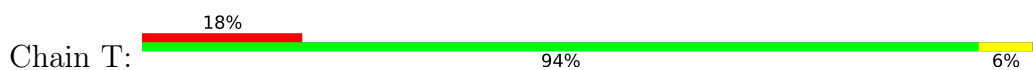
• Molecule 26: 40S ribosomal protein S16-A



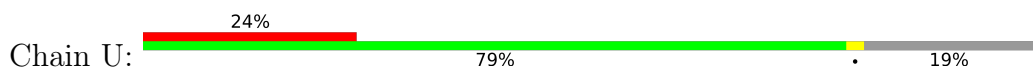
• Molecule 27: 40S ribosomal protein S18-A

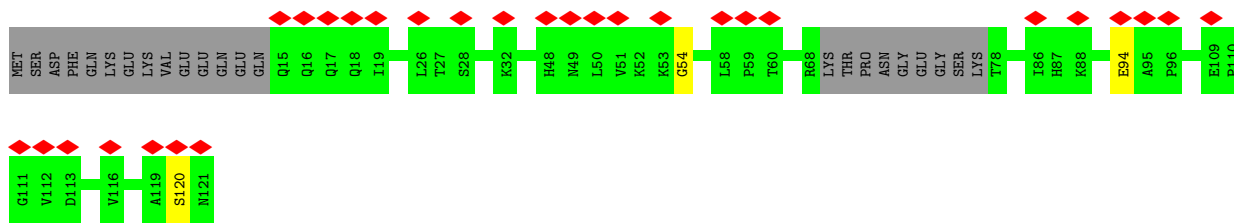


• Molecule 28: 40S ribosomal protein S19-A

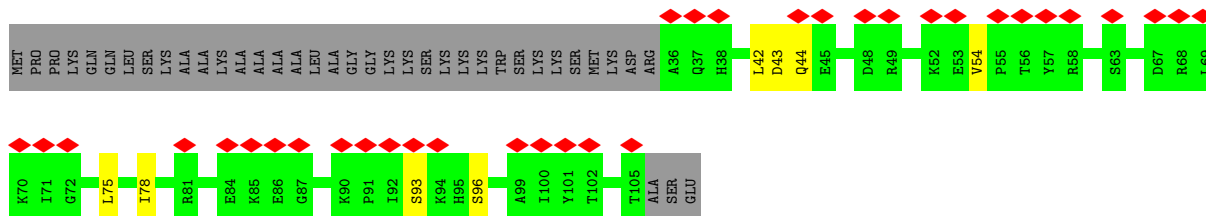


• Molecule 29: 40S ribosomal protein S20

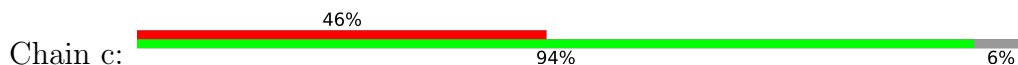




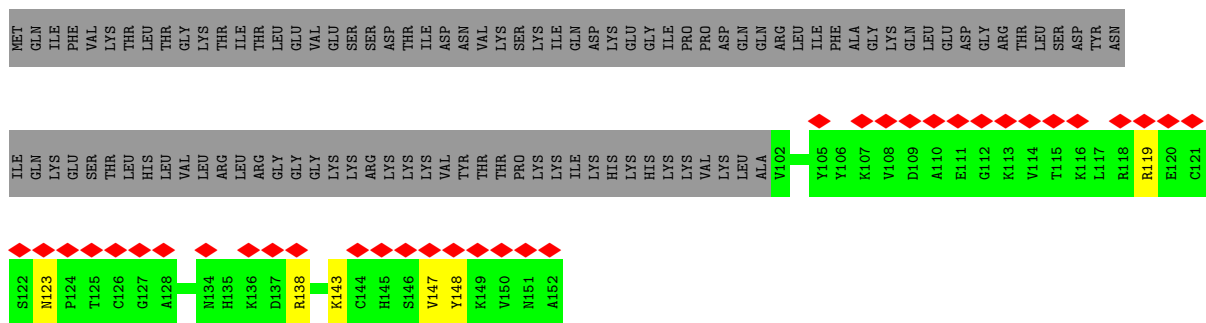
• Molecule 30: 40S ribosomal protein S25-A



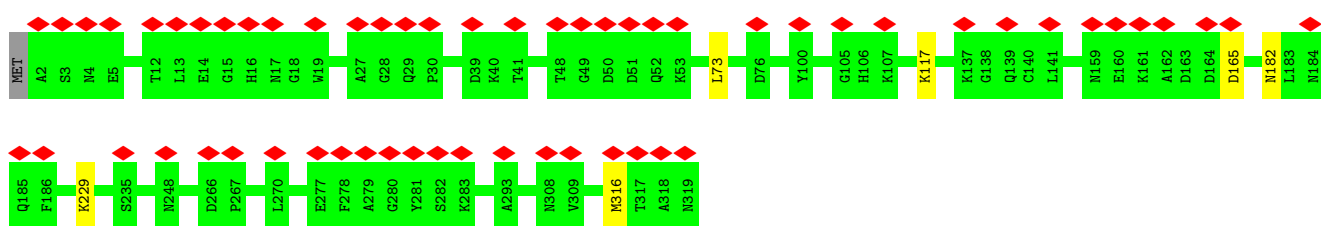
• Molecule 31: 40S ribosomal protein S28-A



• Molecule 32: Ubiquitin-40S ribosomal protein S31



• Molecule 33: Guanine nucleotide-binding protein subunit beta-like protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42901	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 ($e^-/\text{\AA}^2$)	32.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.555	Depositor
Minimum map value	-0.228	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.095	Depositor
Map size (\AA)	409.72803, 409.72803, 409.72803	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.62	2/41697 (0.0%)	1.30	529/64961 (0.8%)
2	A	0.39	0/1617	0.70	0/2215
3	B	0.31	0/929	0.75	0/1250
4	C	0.46	1/1665 (0.1%)	0.68	0/2263
5	E	0.45	0/2109	0.75	1/2839 (0.0%)
6	G	0.40	0/1823	0.69	2/2439 (0.1%)
7	H	0.34	0/1506	0.75	1/2028 (0.0%)
8	I	0.41	0/1514	0.70	1/2021 (0.0%)
9	J	0.42	0/1519	0.74	2/2035 (0.1%)
10	L	0.45	0/1239	0.64	0/1673
11	N	0.33	0/1215	0.71	2/1638 (0.1%)
12	O	0.32	0/142	0.85	0/185
13	R	0.33	0/935	0.78	0/1254
14	V	0.43	0/693	0.79	0/935
15	W	0.49	0/1038	0.73	0/1395
16	X	0.42	0/1139	0.76	1/1518 (0.1%)
17	Y	0.44	0/1087	0.66	0/1449
18	b	0.33	0/620	0.76	0/838
19	d	0.33	0/452	0.61	0/600
20	e	0.34	0/483	0.64	0/643
21	D	0.35	0/1759	0.68	2/2368 (0.1%)
22	F	0.33	0/1629	0.68	1/2202 (0.0%)
23	K	0.39	0/789	0.75	1/1067 (0.1%)
24	M	0.33	0/898	0.93	2/1220 (0.2%)
25	P	0.36	0/998	0.69	0/1341
26	Q	0.33	0/1125	0.81	2/1510 (0.1%)
27	S	0.32	0/1211	0.68	0/1628
28	T	0.44	1/1130 (0.1%)	0.74	1/1517 (0.1%)
29	U	0.30	0/798	0.62	0/1075
30	Z	0.31	0/571	0.81	2/768 (0.3%)
31	c	0.29	0/499	0.62	0/670
32	f	0.35	0/404	0.70	0/542
33	g	0.35	0/2490	0.70	1/3389 (0.0%)
All	All	0.53	4/77723 (0.0%)	1.09	551/113476 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	3
3	B	0	2
4	C	0	4
5	E	0	2
6	G	0	1
7	H	0	4
8	I	0	2
9	J	0	6
11	N	0	4
12	O	0	1
13	R	0	2
14	V	0	4
15	W	0	2
16	X	0	3
17	Y	0	2
21	D	0	2
22	F	0	8
23	K	0	3
24	M	0	8
25	P	0	2
26	Q	0	3
27	S	0	3
28	T	0	2
29	U	0	2
30	Z	0	3
32	f	0	4
33	g	0	1
All	All	0	83

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	53	TRP	CB-CG	6.24	1.61	1.50
4	C	225	LEU	C-N	-6.11	1.20	1.34
1	2	622	A	N9-C4	-5.22	1.34	1.37
1	2	862	A	N9-C4	-5.22	1.34	1.37

All (551) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	934	C	N1-C2-O2	14.62	127.67	118.90
1	2	934	C	C2-N1-C1'	13.01	133.11	118.80
1	2	543	C	N1-C2-O2	12.71	126.53	118.90
1	2	75	U	C2-N1-C1'	12.53	132.73	117.70
26	Q	124	PRO	C-N-CA	11.57	150.63	121.70
1	2	75	U	N1-C2-O2	11.57	130.90	122.80
1	2	794	U	N1-C2-O2	11.46	130.82	122.80
1	2	934	C	N3-C2-O2	-11.33	113.97	121.90
1	2	543	C	N3-C2-O2	-11.01	114.19	121.90
1	2	794	U	N3-C2-O2	-10.97	114.52	122.20
1	2	1363	U	C2-N1-C1'	10.91	130.80	117.70
1	2	1363	U	N1-C2-O2	10.68	130.28	122.80
1	2	75	U	N3-C2-O2	-10.68	114.73	122.20
1	2	1389	C	C2-N1-C1'	10.61	130.47	118.80
1	2	321	C	N1-C2-O2	10.54	125.22	118.90
1	2	794	U	C2-N1-C1'	10.43	130.21	117.70
1	2	192	U	C2-N1-C1'	10.21	129.96	117.70
1	2	192	U	N1-C2-O2	10.19	129.93	122.80
1	2	507	U	N3-C2-O2	-10.18	115.07	122.20
1	2	507	U	N1-C2-O2	9.96	129.77	122.80
33	g	165	ASP	CB-CG-OD1	9.82	127.14	118.30
1	2	1743	U	C2-N1-C1'	9.80	129.46	117.70
1	2	1686	C	C5-C6-N1	9.62	125.81	121.00
1	2	1363	U	N3-C2-O2	-9.61	115.47	122.20
1	2	192	U	N3-C2-O2	-9.55	115.52	122.20
1	2	1398	U	N3-C2-O2	-9.45	115.58	122.20
1	2	1398	U	N1-C2-O2	9.36	129.35	122.80
28	T	35	ASP	CB-CG-OD1	9.31	126.68	118.30
1	2	1162	C	N1-C2-O2	9.30	124.48	118.90
1	2	691	C	C2-N1-C1'	9.19	128.91	118.80
1	2	1246	C	C2-N1-C1'	9.16	128.88	118.80
1	2	1473	U	N1-C2-O2	9.15	129.21	122.80
1	2	1743	U	N1-C2-O2	9.12	129.18	122.80
1	2	1246	C	N1-C2-O2	9.03	124.32	118.90
1	2	453	U	C2-N1-C1'	9.03	128.53	117.70
1	2	484	C	N1-C2-O2	9.02	124.31	118.90
1	2	728	U	N1-C2-O2	9.00	129.10	122.80
1	2	934	C	C6-N1-C1'	-9.00	110.00	120.80
1	2	728	U	C2-N1-C1'	8.92	128.40	117.70
1	2	728	U	N3-C2-O2	-8.91	115.96	122.20
1	2	1458	G	N3-C4-N9	8.83	131.30	126.00
1	2	1743	U	N3-C2-O2	-8.81	116.03	122.20
1	2	934	C	C6-N1-C2	-8.76	116.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1340	U	N1-C2-O2	8.75	128.93	122.80
1	2	1456	C	C2-N1-C1'	8.67	128.34	118.80
1	2	453	U	N1-C2-O2	8.57	128.80	122.80
1	2	864	U	N3-C2-O2	-8.54	116.22	122.20
1	2	507	U	C2-N1-C1'	8.53	127.94	117.70
1	2	543	C	C2-N1-C1'	8.49	128.14	118.80
1	2	1051	G	P-O3'-C3'	8.46	129.85	119.70
1	2	1473	U	C2-N1-C1'	8.38	127.76	117.70
1	2	321	C	C2-N1-C1'	8.35	127.98	118.80
1	2	965	U	C2-N1-C1'	8.35	127.72	117.70
1	2	71	A	C8-N9-C4	-8.32	102.47	105.80
1	2	1473	U	N3-C2-O2	-8.29	116.40	122.20
1	2	639	U	N1-C2-O2	8.28	128.60	122.80
1	2	75	U	C6-N1-C1'	-8.27	109.62	121.20
1	2	1389	C	N1-C2-O2	8.24	123.84	118.90
1	2	1251	U	O5'-P-OP1	-8.19	98.33	105.70
1	2	321	C	N3-C2-O2	-8.18	116.17	121.90
1	2	1307	U	N1-C2-O2	8.15	128.50	122.80
1	2	1652	C	N1-C2-O2	8.14	123.78	118.90
1	2	864	U	N1-C2-O2	8.11	128.48	122.80
1	2	1161	C	C6-N1-C2	-8.09	117.06	120.30
1	2	1389	C	C5-C6-N1	8.07	125.03	121.00
1	2	73	U	O4'-C1'-N1	8.05	114.64	108.20
1	2	184	C	C2-N1-C1'	8.03	127.64	118.80
1	2	453	U	N3-C2-O2	-7.99	116.61	122.20
1	2	1162	C	N3-C2-O2	-7.94	116.34	121.90
1	2	1214	U	N1-C2-O2	7.92	128.34	122.80
1	2	185	U	C2-N1-C1'	7.91	127.19	117.70
1	2	730	G	N3-C4-C5	-7.87	124.66	128.60
1	2	1307	U	C2-N1-C1'	7.86	127.13	117.70
1	2	532	U	C2-N1-C1'	7.84	127.11	117.70
1	2	827	C	N1-C2-O2	7.83	123.60	118.90
1	2	1398	U	C2-N1-C1'	7.74	126.98	117.70
1	2	1458	G	C4-N9-C1'	7.73	136.55	126.50
1	2	1489	U	N3-C2-O2	-7.71	116.80	122.20
1	2	185	U	N1-C2-O2	7.68	128.18	122.80
1	2	1246	C	N3-C2-O2	-7.68	116.52	121.90
1	2	1147	A	C5-C6-N6	-7.67	117.56	123.70
1	2	1258	U	N1-C2-O2	7.64	128.15	122.80
1	2	656	G	O4'-C1'-N9	7.63	114.31	108.20
1	2	1147	A	N1-C6-N6	7.62	123.17	118.60
1	2	730	G	N3-C4-N9	7.57	130.54	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1626	U	C5-C6-N1	7.55	126.48	122.70
1	2	120	U	N3-C2-O2	-7.50	116.95	122.20
1	2	1458	G	N3-C4-C5	-7.49	124.86	128.60
1	2	1591	C	C5-C6-N1	7.49	124.74	121.00
1	2	1162	C	C2-N1-C1'	7.46	127.00	118.80
1	2	1527	C	C2-N1-C1'	7.42	126.97	118.80
1	2	864	U	C2-N1-C1'	7.42	126.61	117.70
1	2	1332	C	C2-N1-C1'	7.42	126.96	118.80
1	2	1456	C	N1-C2-O2	7.41	123.35	118.90
1	2	1393	C	C6-N1-C2	-7.41	117.34	120.30
1	2	1317	C	C6-N1-C2	-7.38	117.35	120.30
1	2	1565	C	C6-N1-C2	-7.37	117.35	120.30
1	2	1332	C	N1-C2-O2	7.35	123.31	118.90
1	2	1646	C	N1-C2-O2	7.35	123.31	118.90
1	2	1626	U	C2-N1-C1'	7.33	126.50	117.70
1	2	758	U	N3-C2-O2	-7.33	117.07	122.20
1	2	558	U	C2-N1-C1'	7.32	126.49	117.70
1	2	1340	U	N3-C2-O2	-7.32	117.08	122.20
1	2	116	U	N3-C2-O2	-7.31	117.08	122.20
1	2	1389	C	C6-N1-C1'	-7.30	112.04	120.80
1	2	1596	C	C2-N1-C1'	7.29	126.82	118.80
1	2	1161	C	C2-N1-C1'	7.28	126.81	118.80
1	2	1489	U	C2-N1-C1'	7.28	126.43	117.70
1	2	1220	C	C5-C6-N1	7.28	124.64	121.00
1	2	1051	G	OP1-P-O3'	7.27	121.19	105.20
1	2	1363	U	C6-N1-C1'	-7.27	111.03	121.20
1	2	1252	C	C5-C6-N1	7.26	124.63	121.00
1	2	224	C	C5-C6-N1	7.26	124.63	121.00
1	2	491	C	N1-C2-O2	7.25	123.25	118.90
1	2	1252	C	C6-N1-C2	-7.24	117.40	120.30
1	2	1340	U	C2-N1-C1'	7.20	126.34	117.70
1	2	558	U	C5-C6-N1	7.20	126.30	122.70
1	2	831	U	N3-C2-O2	-7.19	117.17	122.20
1	2	497	G	P-O3'-C3'	7.19	128.32	119.70
1	2	758	U	N1-C2-O2	7.18	127.83	122.80
1	2	1258	U	N3-C2-O2	-7.16	117.19	122.20
1	2	185	U	N3-C2-O2	-7.16	117.19	122.20
1	2	1274	C	C2-N1-C1'	7.15	126.66	118.80
1	2	831	U	C2-N1-C1'	7.13	126.26	117.70
1	2	241	U	O5'-P-OP2	-7.13	99.28	105.70
1	2	1161	C	C5-C6-N1	7.13	124.56	121.00
1	2	1527	C	N1-C2-O2	7.13	123.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1560	U	C2-N1-C1'	7.11	126.23	117.70
1	2	1657	U	N3-C2-O2	-7.11	117.22	122.20
1	2	1327	C	C6-N1-C2	-7.11	117.46	120.30
1	2	184	C	C5-C6-N1	7.09	124.55	121.00
1	2	1393	C	C5-C6-N1	7.08	124.54	121.00
1	2	1686	C	C6-N1-C2	-7.08	117.47	120.30
1	2	1370	U	P-O3'-C3'	7.06	128.17	119.70
1	2	1489	U	N1-C2-O2	7.06	127.74	122.80
1	2	1389	C	C6-N1-C2	-7.05	117.48	120.30
23	K	40	LEU	CA-CB-CG	7.03	131.47	115.30
1	2	639	U	C2-N1-C1'	7.02	126.13	117.70
1	2	1307	U	N3-C2-O2	-7.02	117.29	122.20
1	2	831	U	N1-C2-O2	7.01	127.70	122.80
1	2	934	C	C5-C6-N1	7.00	124.50	121.00
1	2	1197	C	N1-C2-O2	6.98	123.09	118.90
1	2	639	U	N3-C2-O2	-6.97	117.32	122.20
1	2	721	U	O5'-P-OP1	-6.97	99.43	105.70
1	2	500	C	C5-C4-N4	-6.97	115.32	120.20
1	2	691	C	N1-C2-O2	6.97	123.08	118.90
1	2	782	U	OP2-P-O3'	6.96	120.51	105.20
1	2	1246	C	C6-N1-C2	-6.96	117.52	120.30
1	2	1258	U	C2-N1-C1'	6.96	126.05	117.70
1	2	559	C	C2-N1-C1'	6.93	126.42	118.80
22	F	58	LEU	CA-CB-CG	6.90	131.18	115.30
1	2	1279	C	C6-N1-C2	-6.89	117.54	120.30
1	2	1596	C	N1-C2-O2	6.89	123.04	118.90
1	2	484	C	N3-C2-O2	-6.89	117.08	121.90
1	2	1115	U	N1-C2-O2	6.89	127.62	122.80
1	2	1211	A	N7-C8-N9	6.88	117.24	113.80
1	2	1214	U	N3-C2-O2	-6.87	117.39	122.20
1	2	1709	C	N1-C2-O2	6.87	123.02	118.90
24	M	36	LEU	CA-CB-CG	6.85	131.05	115.30
1	2	1000	C	C2-N1-C1'	6.84	126.32	118.80
1	2	1560	U	N1-C2-O2	6.82	127.58	122.80
1	2	648	G	N3-C4-N9	6.81	130.09	126.00
1	2	1688	U	C5-C6-N1	6.81	126.10	122.70
1	2	720	G	C4-N9-C1'	6.80	135.34	126.50
1	2	1012	U	C5-C4-O4	-6.78	121.83	125.90
1	2	827	C	N3-C2-O2	-6.78	117.16	121.90
1	2	1012	U	N3-C4-O4	6.77	124.14	119.40
1	2	782	U	P-O3'-C3'	6.76	127.82	119.70
1	2	730	G	C4-N9-C1'	6.75	135.28	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1664	C	C2-N1-C1'	6.75	126.22	118.80
1	2	508	U	N1-C2-O2	6.74	127.52	122.80
1	2	185	U	C5-C6-N1	6.73	126.06	122.70
1	2	1527	C	C6-N1-C2	-6.72	117.61	120.30
1	2	75	U	C5-C6-N1	6.71	126.06	122.70
1	2	120	U	N1-C2-O2	6.70	127.49	122.80
1	2	1000	C	N1-C2-O2	6.70	122.92	118.90
1	2	1115	U	N3-C2-O2	-6.70	117.51	122.20
1	2	1000	C	N3-C2-O2	-6.70	117.21	121.90
1	2	1205	C	N1-C2-O2	6.70	122.92	118.90
1	2	1458	G	C8-N9-C1'	-6.69	118.31	127.00
26	Q	53	LEU	CA-CB-CG	-6.69	99.92	115.30
1	2	1210	C	C6-N1-C2	-6.67	117.63	120.30
1	2	656	G	C4-N9-C1'	-6.67	117.83	126.50
1	2	1379	C	N1-C2-O2	6.66	122.89	118.90
1	2	1497	U	N1-C2-O2	6.64	127.45	122.80
1	2	965	U	C6-N1-C1'	-6.61	111.94	121.20
1	2	648	G	C4-N9-C1'	6.61	135.09	126.50
1	2	543	C	C6-N1-C2	-6.60	117.66	120.30
1	2	1301	U	N1-C2-O2	6.60	127.42	122.80
1	2	777	C	C2-N1-C1'	6.59	126.05	118.80
1	2	139	C	P-O3'-C3'	6.56	127.57	119.70
1	2	1000	C	C6-N1-C2	-6.55	117.68	120.30
1	2	1454	G	N1-C6-O6	-6.55	115.97	119.90
1	2	691	C	C6-N1-C1'	-6.55	112.94	120.80
1	2	992	A	C8-N9-C4	-6.55	103.18	105.80
1	2	794	U	C6-N1-C1'	-6.54	112.04	121.20
1	2	1293	U	N3-C2-O2	-6.53	117.63	122.20
1	2	1399	C	C6-N1-C2	-6.52	117.69	120.30
1	2	71	A	N7-C8-N9	6.52	117.06	113.80
1	2	992	A	N9-C4-C5	6.51	108.41	105.80
1	2	1302	U	N3-C2-O2	-6.50	117.65	122.20
1	2	484	C	C2-N1-C1'	6.50	125.95	118.80
11	N	21	ASN	C-N-CA	6.50	137.94	121.70
1	2	192	U	C6-N1-C1'	-6.48	112.12	121.20
1	2	192	U	C5-C6-N1	6.48	125.94	122.70
1	2	1273	G	N3-C4-N9	-6.47	122.12	126.00
1	2	532	U	N3-C2-O2	-6.47	117.67	122.20
1	2	1279	C	C5-C6-N1	6.46	124.23	121.00
1	2	1646	C	N3-C2-O2	-6.46	117.38	121.90
1	2	1302	U	N1-C2-O2	6.45	127.32	122.80
1	2	725	U	N3-C2-O2	-6.45	117.69	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1646	C	C2-N1-C1'	6.44	125.89	118.80
1	2	700	C	C6-N1-C2	-6.44	117.73	120.30
1	2	959	U	N1-C2-O2	6.42	127.30	122.80
1	2	1657	U	N1-C2-O2	6.42	127.30	122.80
1	2	1742	U	N3-C2-O2	-6.40	117.72	122.20
1	2	74	U	O5'-P-OP1	-6.39	99.94	105.70
1	2	1215	C	C5-C6-N1	6.39	124.20	121.00
1	2	1301	U	C2-N1-C1'	6.36	125.33	117.70
1	2	829	A	P-O3'-C3'	6.35	127.32	119.70
1	2	79	C	C6-N1-C2	-6.34	117.76	120.30
1	2	532	U	N1-C2-O2	6.34	127.24	122.80
1	2	184	C	C6-N1-C2	-6.34	117.77	120.30
1	2	1566	U	C5-C6-N1	6.33	125.87	122.70
1	2	1280	C	C5-C6-N1	6.33	124.17	121.00
1	2	720	G	N3-C4-N9	6.32	129.79	126.00
1	2	767	U	N3-C2-O2	-6.32	117.77	122.20
1	2	267	U	N3-C2-O2	-6.31	117.78	122.20
1	2	794	U	P-O3'-C3'	6.31	127.27	119.70
1	2	656	G	C8-N9-C1'	6.31	135.20	127.00
1	2	1280	C	C6-N1-C2	-6.30	117.78	120.30
1	2	648	G	C8-N9-C1'	-6.29	118.82	127.00
1	2	500	C	N3-C4-N4	6.29	122.40	118.00
1	2	501	U	P-O3'-C3'	6.29	127.24	119.70
1	2	990	C	C5-C6-N1	6.29	124.14	121.00
6	G	68	LEU	CB-CG-CD2	6.28	121.68	111.00
1	2	794	U	C5-C6-N1	6.28	125.84	122.70
1	2	1214	U	C2-N1-C1'	6.24	125.19	117.70
1	2	1440	C	C2-N1-C1'	6.22	125.64	118.80
1	2	1060	U	N3-C2-O2	-6.22	117.85	122.20
1	2	1295	G	C8-N9-C4	-6.20	103.92	106.40
1	2	223	U	N1-C2-O2	6.20	127.14	122.80
1	2	1510	U	N1-C2-O2	6.19	127.14	122.80
1	2	558	U	N1-C2-O2	6.19	127.13	122.80
1	2	704	C	N1-C2-O2	6.18	122.61	118.90
1	2	1560	U	N3-C2-O2	-6.18	117.88	122.20
1	2	990	C	C6-N1-C2	-6.18	117.83	120.30
1	2	158	U	P-O3'-C3'	6.16	127.09	119.70
1	2	1743	U	C6-N1-C1'	-6.15	112.59	121.20
1	2	1147	A	C4-C5-N7	6.14	113.77	110.70
1	2	1652	C	C2-N1-C1'	6.14	125.56	118.80
1	2	508	U	N3-C2-O2	-6.14	117.90	122.20
1	2	1440	C	N1-C2-O2	6.14	122.58	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	777	C	N1-C2-O2	6.13	122.58	118.90
1	2	158	U	OP1-P-O3'	6.12	118.67	105.20
1	2	74	U	C5-C6-N1	6.12	125.76	122.70
1	2	1289	U	N1-C2-O2	6.11	127.08	122.80
1	2	1414	U	N1-C2-O2	6.10	127.07	122.80
24	M	103	LEU	CA-CB-CG	6.09	129.32	115.30
1	2	1573	A	P-O3'-C3'	6.09	127.01	119.70
1	2	965	U	N1-C2-O2	6.09	127.06	122.80
1	2	1296	A	N7-C8-N9	6.08	116.84	113.80
1	2	927	C	N3-C2-O2	-6.07	117.65	121.90
1	2	1456	C	N3-C2-O2	-6.06	117.66	121.90
1	2	497	G	OP1-P-O3'	6.06	118.53	105.20
1	2	729	G	C4-N9-C1'	6.05	134.37	126.50
1	2	1220	C	C6-N1-C2	-6.05	117.88	120.30
1	2	725	U	N1-C2-O2	6.04	127.03	122.80
1	2	1664	C	N1-C2-O2	6.04	122.52	118.90
1	2	959	U	C2-N1-C1'	6.03	124.94	117.70
1	2	283	U	N1-C2-O2	6.03	127.02	122.80
1	2	934	C	C2-N3-C4	6.03	122.92	119.90
1	2	1573	A	OP2-P-O3'	6.03	118.46	105.20
1	2	862	A	C8-N9-C4	6.02	108.21	105.80
1	2	1646	C	C6-N1-C2	-6.02	117.89	120.30
1	2	700	C	N1-C2-O2	6.01	122.51	118.90
1	2	1147	A	N9-C4-C5	-6.01	103.39	105.80
1	2	1339	C	OP2-P-O3'	6.00	118.41	105.20
1	2	1246	C	C6-N1-C1'	-6.00	113.60	120.80
1	2	1596	C	N3-C2-O2	-6.00	117.70	121.90
1	2	502	U	C5-C6-N1	5.99	125.69	122.70
1	2	453	U	C6-N1-C1'	-5.98	112.83	121.20
1	2	1147	A	C6-C5-N7	-5.97	128.12	132.30
1	2	720	G	C8-N9-C1'	-5.97	119.24	127.00
1	2	959	U	N3-C2-O2	-5.97	118.02	122.20
1	2	1743	U	C5-C6-N1	5.97	125.69	122.70
1	2	1363	U	C5-C6-N1	5.96	125.68	122.70
1	2	1185	U	N1-C2-O2	5.96	126.97	122.80
1	2	1715	G	N3-C4-N9	5.95	129.57	126.00
1	2	1456	C	C6-N1-C1'	-5.95	113.67	120.80
1	2	491	C	N3-C2-O2	-5.94	117.74	121.90
1	2	1510	U	N3-C2-O2	-5.93	118.05	122.20
1	2	755	A	P-O3'-C3'	5.93	126.81	119.70
1	2	1021	C	N1-C2-O2	5.93	122.46	118.90
1	2	1652	C	N3-C2-O2	-5.92	117.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1567	U	N1-C2-O2	5.90	126.93	122.80
1	2	1225	U	N3-C2-O2	-5.89	118.07	122.20
1	2	831	U	C5-C6-N1	5.89	125.64	122.70
1	2	500	C	C5-C6-N1	5.89	123.94	121.00
1	2	767	U	N1-C2-O2	5.89	126.92	122.80
1	2	1474	G	N1-C6-O6	-5.89	116.37	119.90
9	J	93	LEU	CA-CB-CG	5.89	128.85	115.30
1	2	1398	U	C5-C6-N1	5.88	125.64	122.70
1	2	1567	U	N3-C2-O2	-5.88	118.08	122.20
1	2	280	U	P-O3'-C3'	5.88	126.76	119.70
1	2	1389	C	N3-C2-O2	-5.88	117.78	121.90
1	2	767	U	C2-N1-C1'	5.88	124.75	117.70
1	2	1185	U	C2-N1-C1'	5.88	124.75	117.70
1	2	1060	U	N1-C2-O2	5.87	126.91	122.80
1	2	270	C	C2-N1-C1'	5.87	125.25	118.80
1	2	1225	U	N1-C2-O2	5.86	126.91	122.80
1	2	79	C	C2-N1-C1'	5.85	125.23	118.80
1	2	490	C	N1-C2-O2	5.84	122.40	118.90
1	2	581	U	C2-N1-C1'	5.84	124.71	117.70
1	2	1591	C	C6-N1-C2	-5.84	117.97	120.30
1	2	1742	U	N1-C2-O2	5.84	126.89	122.80
1	2	25	C	C6-N1-C2	5.83	122.63	120.30
1	2	1770	U	N1-C2-O2	5.83	126.88	122.80
1	2	302	U	N3-C2-O2	-5.82	118.12	122.20
1	2	1414	U	C2-N1-C1'	5.81	124.67	117.70
1	2	1497	U	N3-C2-O2	-5.81	118.14	122.20
1	2	721	U	P-O3'-C3'	5.80	126.66	119.70
11	N	88	LEU	CA-CB-CG	5.80	128.64	115.30
1	2	1196	A	P-O3'-C3'	5.79	126.65	119.70
1	2	1398	U	C6-N1-C2	-5.78	117.53	121.00
1	2	1197	C	C6-N1-C2	-5.77	117.99	120.30
21	D	93	ASP	CB-CG-OD1	5.77	123.49	118.30
1	2	783	G	C3'-C2'-C1'	5.77	106.11	101.50
1	2	1305	U	N1-C2-O2	5.77	126.84	122.80
1	2	1317	C	C5-C6-N1	5.77	123.89	121.00
1	2	996	U	C2-N1-C1'	5.77	124.62	117.70
1	2	1456	C	C6-N1-C2	-5.77	117.99	120.30
1	2	321	C	C6-N1-C2	-5.76	117.99	120.30
1	2	1305	U	N3-C2-O2	-5.76	118.17	122.20
1	2	1474	G	N9-C4-C5	5.76	107.70	105.40
1	2	1197	C	C5-C6-N1	5.76	123.88	121.00
1	2	1295	G	N7-C8-N9	5.75	115.98	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1063	U	C5-C6-N1	5.75	125.57	122.70
1	2	730	G	C2-N3-C4	5.75	114.77	111.90
1	2	1162	C	C6-N1-C2	-5.73	118.01	120.30
1	2	1305	U	C2-N1-C1'	5.73	124.58	117.70
1	2	1596	C	C6-N1-C2	-5.72	118.01	120.30
1	2	1052	U	C2-N1-C1'	5.71	124.55	117.70
1	2	1148	C	C5-C6-N1	5.70	123.85	121.00
1	2	1476	C	C6-N1-C2	-5.70	118.02	120.30
1	2	691	C	C5-C6-N1	5.70	123.85	121.00
1	2	1665	U	C5-C6-N1	5.70	125.55	122.70
1	2	1060	U	C2-N1-C1'	5.69	124.53	117.70
1	2	559	C	N1-C2-O2	5.68	122.31	118.90
1	2	1568	C	P-O3'-C3'	5.68	126.52	119.70
30	Z	75	LEU	CA-CB-CG	5.68	128.37	115.30
1	2	1161	C	N1-C2-O2	5.68	122.31	118.90
1	2	691	C	C6-N1-C2	-5.67	118.03	120.30
1	2	321	C	C6-N1-C1'	-5.67	114.00	120.80
1	2	827	C	O4'-C1'-N1	5.67	112.74	108.20
1	2	1440	C	C5-C6-N1	5.67	123.84	121.00
1	2	720	G	N3-C4-C5	-5.67	125.77	128.60
1	2	653	C	C6-N1-C2	-5.67	118.03	120.30
1	2	1542	G	O4'-C1'-N9	5.67	112.73	108.20
1	2	781	U	P-O3'-C3'	5.66	126.50	119.70
1	2	417	A	P-O3'-C3'	5.66	126.49	119.70
1	2	1274	C	N1-C2-O2	5.66	122.30	118.90
1	2	1379	C	N3-C2-O2	-5.66	117.94	121.90
1	2	278	U	P-O3'-C3'	5.66	126.49	119.70
1	2	1734	U	P-O3'-C3'	5.66	126.49	119.70
1	2	74	U	C6-N1-C2	-5.66	117.61	121.00
1	2	728	U	C6-N1-C1'	-5.66	113.28	121.20
1	2	1644	C	C6-N1-C2	-5.65	118.04	120.30
1	2	149	C	C2-N1-C1'	5.65	125.01	118.80
1	2	1454	G	C5-C6-O6	5.63	131.98	128.60
6	G	68	LEU	CA-CB-CG	5.63	128.26	115.30
1	2	1205	C	N3-C2-O2	-5.63	117.96	121.90
1	2	581	U	N1-C2-O2	5.62	126.74	122.80
1	2	730	G	C8-N9-C1'	-5.62	119.70	127.00
1	2	1664	C	C6-N1-C2	-5.62	118.05	120.30
1	2	1661	U	N3-C2-O2	-5.62	118.27	122.20
1	2	1609	U	N3-C2-O2	-5.60	118.28	122.20
1	2	720	G	P-O3'-C3'	5.60	126.42	119.70
1	2	1739	C	N1-C2-O2	5.60	122.26	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	823	G	C2-N3-C4	5.59	114.70	111.90
1	2	1708	U	N1-C2-O2	5.59	126.72	122.80
1	2	1527	C	C5-C6-N1	5.59	123.79	121.00
1	2	75	U	C6-N1-C2	-5.59	117.65	121.00
1	2	583	C	C5-C6-N1	5.59	123.79	121.00
1	2	1770	U	N3-C2-O2	-5.59	118.29	122.20
1	2	70	C	N3-C2-O2	-5.58	117.99	121.90
1	2	1244	A	P-O3'-C3'	5.58	126.40	119.70
1	2	1399	C	N1-C2-O2	5.58	122.25	118.90
1	2	223	U	N3-C2-O2	-5.57	118.30	122.20
1	2	283	U	N3-C2-O2	-5.57	118.30	122.20
1	2	224	C	C6-N1-C2	-5.57	118.07	120.30
1	2	1414	U	N3-C2-O2	-5.56	118.31	122.20
1	2	1709	C	N3-C2-O2	-5.56	118.01	121.90
1	2	1293	U	N1-C2-O2	5.56	126.69	122.80
1	2	1743	U	C6-N1-C2	-5.55	117.67	121.00
1	2	1686	C	C2-N1-C1'	5.55	124.90	118.80
1	2	581	U	N3-C2-O2	-5.55	118.32	122.20
1	2	725	U	C2-N1-C1'	5.55	124.36	117.70
1	2	1197	C	N3-C2-O2	-5.55	118.02	121.90
1	2	1246	C	C5-C6-N1	5.54	123.77	121.00
1	2	1226	A	P-O3'-C3'	5.53	126.34	119.70
1	2	1723	U	N1-C2-O2	5.53	126.67	122.80
1	2	1299	G	O5'-P-OP2	-5.52	100.73	105.70
1	2	184	C	N1-C2-O2	5.52	122.21	118.90
1	2	1567	U	C5-C6-N1	5.51	125.46	122.70
1	2	543	C	C6-N1-C1'	-5.51	114.19	120.80
1	2	490	C	N3-C2-O2	-5.51	118.05	121.90
7	H	166	LEU	CA-CB-CG	5.50	127.96	115.30
1	2	267	U	N1-C2-O2	5.50	126.65	122.80
1	2	218	A	C2-N3-C4	5.50	113.35	110.60
1	2	1080	U	N1-C2-O2	5.50	126.65	122.80
1	2	685	A	P-O3'-C3'	5.49	126.29	119.70
1	2	700	C	N3-C2-O2	-5.49	118.06	121.90
1	2	1301	U	N3-C2-O2	-5.48	118.36	122.20
1	2	996	U	N1-C2-O2	5.47	126.63	122.80
1	2	189	C	N1-C2-O2	5.47	122.18	118.90
1	2	1473	U	C6-N1-C1'	-5.47	113.55	121.20
1	2	694	U	N3-C2-O2	-5.46	118.37	122.20
1	2	1012	U	N1-C2-O2	5.46	126.62	122.80
1	2	142	G	N3-C2-N2	-5.46	116.08	119.90
9	J	118	LEU	CA-CB-CG	5.45	127.84	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	558	U	N3-C2-O2	-5.45	118.39	122.20
1	2	945	U	N1-C2-O2	5.45	126.61	122.80
1	2	35	U	N1-C2-O2	5.43	126.60	122.80
1	2	1063	U	C2-N1-C1'	5.43	124.22	117.70
1	2	1708	U	N3-C2-O2	-5.43	118.40	122.20
1	2	131	C	P-O3'-C3'	5.43	126.21	119.70
1	2	794	U	C6-N1-C2	-5.43	117.74	121.00
1	2	1395	G	N3-C4-N9	5.41	129.25	126.00
1	2	1629	G	N3-C2-N2	5.41	123.68	119.90
1	2	826	U	C2-N1-C1'	5.40	124.18	117.70
1	2	1161	C	C2-N3-C4	5.40	122.60	119.90
1	2	1759	C	C6-N1-C2	-5.40	118.14	120.30
1	2	79	C	C5-C6-N1	5.40	123.70	121.00
1	2	826	U	N3-C2-O2	-5.40	118.42	122.20
1	2	722	G	N3-C4-C5	-5.39	125.91	128.60
1	2	1657	U	C5-C6-N1	5.38	125.39	122.70
1	2	996	U	N3-C2-O2	-5.38	118.43	122.20
1	2	35	U	N3-C2-O2	-5.38	118.44	122.20
1	2	747	C	C2-N1-C1'	5.38	124.72	118.80
1	2	1052	U	N1-C2-O2	5.37	126.56	122.80
1	2	61	A	O4'-C1'-N9	5.37	112.49	108.20
1	2	192	U	C6-N1-C2	-5.37	117.78	121.00
1	2	1527	C	N3-C2-O2	-5.37	118.14	121.90
1	2	1651	A	C2-N3-C4	5.36	113.28	110.60
8	I	141	ARG	CB-CG-CD	-5.36	97.67	111.60
1	2	1007	C	C6-N1-C2	-5.36	118.16	120.30
1	2	841	U	N3-C2-O2	-5.35	118.45	122.20
1	2	1340	U	O5'-P-OP2	-5.34	100.89	105.70
5	E	38	LEU	CA-CB-CG	5.34	127.58	115.30
1	2	1458	G	C6-C5-N7	-5.34	127.20	130.40
1	2	1530	C	O4'-C1'-N1	5.33	112.46	108.20
1	2	729	G	N3-C4-N9	5.32	129.19	126.00
1	2	1560	U	O4'-C1'-N1	5.32	112.45	108.20
1	2	507	U	C6-N1-C1'	-5.31	113.76	121.20
1	2	1510	U	C2-N1-C1'	5.31	124.08	117.70
1	2	184	C	C6-N1-C1'	-5.31	114.43	120.80
1	2	1638	G	C4-N9-C1'	5.30	133.39	126.50
1	2	720	G	OP1-P-O3'	5.29	116.84	105.20
1	2	1154	G	C4-N9-C1'	5.29	133.38	126.50
1	2	453	U	C5-C6-N1	5.29	125.34	122.70
1	2	737	A	O4'-C1'-N9	5.29	112.43	108.20
1	2	1752	U	C2-N1-C1'	5.29	124.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	136	C	N1-C2-O2	5.28	122.07	118.90
1	2	826	U	N1-C2-O2	5.28	126.50	122.80
1	2	163	G	C4-N9-C1'	5.28	133.36	126.50
1	2	722	G	N3-C4-N9	5.28	129.17	126.00
1	2	1723	U	N3-C2-O2	-5.28	118.50	122.20
1	2	1452	U	C5-C6-N1	5.28	125.34	122.70
1	2	845	G	O4'-C1'-N9	5.27	112.42	108.20
1	2	945	U	N3-C2-O2	-5.27	118.51	122.20
1	2	1185	U	N3-C2-O2	-5.27	118.51	122.20
1	2	1220	C	C2-N1-C1'	5.27	124.60	118.80
16	X	96	VAL	C-N-CA	5.27	134.87	121.70
1	2	1474	G	C5-C6-O6	5.26	131.76	128.60
1	2	1399	C	C5-C6-N1	5.25	123.63	121.00
1	2	1274	C	C6-N1-C1'	-5.25	114.50	120.80
1	2	704	C	N3-C2-O2	-5.25	118.23	121.90
1	2	857	U	N3-C2-O2	-5.25	118.53	122.20
1	2	1635	A	C4-N9-C1'	5.25	135.74	126.30
1	2	1307	U	C6-N1-C1'	-5.24	113.86	121.20
1	2	1121	C	C5-C6-N1	5.24	123.62	121.00
1	2	1603	U	N3-C2-O2	-5.24	118.53	122.20
1	2	321	C	C5-C6-N1	5.23	123.61	121.00
30	Z	96	SER	C-N-CA	5.23	134.78	121.70
1	2	1317	C	C2-N1-C1'	5.22	124.55	118.80
1	2	163	G	C8-N9-C1'	-5.22	120.21	127.00
1	2	1147	A	C5-N7-C8	-5.21	101.30	103.90
1	2	558	U	C6-N1-C2	-5.20	117.88	121.00
1	2	50	C	C2-N1-C1'	5.20	124.52	118.80
1	2	729	G	C8-N9-C1'	-5.20	120.25	127.00
1	2	1456	C	O4'-C1'-N1	5.19	112.35	108.20
1	2	500	C	C6-N1-C2	-5.19	118.22	120.30
1	2	323	A	O5'-P-OP2	-5.19	101.03	105.70
1	2	857	U	N1-C2-O2	5.19	126.43	122.80
1	2	794	U	O4'-C1'-N1	-5.18	104.05	108.20
1	2	94	U	N3-C2-O2	-5.18	118.57	122.20
1	2	587	C	C5-C6-N1	5.17	123.58	121.00
1	2	1228	G	N7-C8-N9	5.17	115.68	113.10
1	2	841	U	N1-C2-O2	5.16	126.41	122.80
1	2	736	C	N3-C2-O2	-5.15	118.29	121.90
1	2	1332	C	C5-C6-N1	5.15	123.58	121.00
1	2	1620	C	N1-C2-O2	5.15	121.99	118.90
1	2	583	C	C2-N1-C1'	5.14	124.46	118.80
1	2	830	U	C2-N1-C1'	5.14	123.87	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1301	U	C5-C6-N1	5.13	125.27	122.70
1	2	1439	C	N1-C2-O2	5.13	121.98	118.90
1	2	1571	C	C6-N1-C2	-5.13	118.25	120.30
1	2	648	G	N3-C4-C5	-5.12	126.04	128.60
1	2	1566	U	C6-N1-C2	-5.12	117.93	121.00
1	2	559	C	C6-N1-C2	-5.12	118.25	120.30
1	2	1257	U	C2-N1-C1'	5.12	123.84	117.70
1	2	361	C	C6-N1-C2	-5.11	118.25	120.30
1	2	804	A	C2-N3-C4	5.11	113.16	110.60
1	2	1012	U	C5-C6-N1	5.11	125.26	122.70
1	2	131	C	OP1-P-O3'	5.11	116.44	105.20
1	2	1289	U	N3-C2-O2	-5.11	118.62	122.20
1	2	270	C	N1-C2-O2	5.11	121.97	118.90
1	2	784	C	C5-C6-N1	5.11	123.55	121.00
1	2	103	A	P-O3'-C3'	5.11	125.83	119.70
1	2	1626	U	N1-C2-O2	5.10	126.37	122.80
1	2	950	C	C6-N1-C2	-5.09	118.26	120.30
1	2	27	U	C5-C6-N1	5.09	125.24	122.70
1	2	627	C	C6-N1-C2	-5.08	118.27	120.30
1	2	1566	U	N3-C2-O2	-5.08	118.64	122.20
1	2	1439	C	C2-N1-C1'	5.08	124.39	118.80
1	2	1379	C	C2-N1-C1'	5.07	124.38	118.80
1	2	1566	U	N1-C2-O2	5.07	126.35	122.80
1	2	1063	U	N1-C2-O2	5.07	126.35	122.80
1	2	1629	G	N3-C4-N9	5.07	129.04	126.00
21	D	4	LEU	CA-CB-CG	5.06	126.95	115.30
1	2	519	C	N1-C2-O2	5.06	121.94	118.90
1	2	1250	U	OP1-P-O3'	5.05	116.32	105.20
1	2	1458	G	C2-N3-C4	5.05	114.43	111.90
1	2	1624	C	C6-N1-C2	-5.05	118.28	120.30
1	2	1332	C	C6-N1-C1'	-5.05	114.74	120.80
1	2	1332	C	C6-N1-C2	-5.05	118.28	120.30
1	2	1738	U	N3-C2-O2	-5.04	118.67	122.20
1	2	824	G	C4-N9-C1'	-5.04	119.95	126.50
1	2	1591	C	C2-N1-C1'	5.04	124.34	118.80
1	2	1202	A	C2-N3-C4	5.04	113.12	110.60
1	2	1627	U	N3-C2-O2	-5.04	118.67	122.20
1	2	532	U	C6-N1-C1'	-5.03	114.15	121.20
1	2	888	U	C5-C6-N1	5.03	125.22	122.70
1	2	212	U	N1-C2-O2	5.03	126.32	122.80
1	2	862	A	N7-C8-N9	-5.03	111.28	113.80
1	2	992	A	N1-C6-N6	-5.03	115.58	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	992	A	N1-C2-N3	5.02	131.81	129.30
1	2	1395	G	C4-N9-C1'	5.01	133.01	126.50
1	2	205	U	N3-C2-O2	-5.01	118.69	122.20
1	2	411	C	C6-N1-C2	-5.01	118.30	120.30

There are no chirality outliers.

All (83) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	166	GLY	Peptide
2	A	3	LEU	Peptide
2	A	94	GLY	Peptide
3	B	147	ALA	Peptide
3	B	206	PRO	Peptide
4	C	144	TRP	Peptide
4	C	87	GLN	Peptide
4	C	90	THR	Peptide
4	C	91	ARG	Peptide
21	D	216	PRO	Peptide
21	D	219	ALA	Peptide
5	E	193	GLY	Peptide
5	E	194	THR	Peptide
22	F	125	THR	Peptide
22	F	127	GLN	Peptide
22	F	128	ASN	Peptide
22	F	44	ASN	Peptide
22	F	49	GLU	Peptide
22	F	56	ALA	Peptide
22	F	57	SER	Peptide
22	F	65	ARG	Peptide
6	G	148	SER	Peptide
7	H	131	PHE	Peptide
7	H	133	THR	Peptide
7	H	64	VAL	Peptide
7	H	97	ARG	Peptide
8	I	151	LYS	Peptide
8	I	8	ARG	Peptide
9	J	117	GLY	Peptide
9	J	161	THR	Peptide
9	J	162	SER	Peptide
9	J	163	PRO	Peptide
9	J	98	ALA	Peptide

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Mol	Chain	Res	Type	Group
9	J	99	LEU	Peptide
23	K	53	GLY	Peptide
23	K	86	ILE	Peptide
23	K	87	VAL	Peptide
24	M	105	LYS	Peptide
24	M	108	ARG	Peptide
24	M	111	ASN	Peptide
24	M	129	GLU	Peptide
24	M	130	THR	Peptide
24	M	41	LEU	Peptide
24	M	84	ASN	Peptide
24	M	89	ILE	Peptide
11	N	137	PRO	Peptide
11	N	21	ASN	Peptide
11	N	22	ALA	Peptide
11	N	24	ALA	Peptide
12	O	123	SER	Peptide
25	P	11	VAL	Peptide
25	P	124	THR	Peptide
26	Q	13	LYS	Peptide
26	Q	40	GLU	Peptide
26	Q	58	ASP	Peptide
13	R	23	LYS	Peptide
13	R	87	GLU	Peptide
27	S	62	THR	Peptide
27	S	90	ASN	Peptide
27	S	91	ASP	Peptide
28	T	30	VAL	Peptide
28	T	52	GLY	Peptide
29	U	54	GLY	Peptide
29	U	94	GLU	Peptide
14	V	50	TYR	Peptide
14	V	79	LEU	Peptide
14	V	80	LYS	Peptide
14	V	81	ASN	Peptide
15	W	29	PRO	Peptide
15	W	82	LYS	Peptide
16	X	137	LYS	Peptide
16	X	88	PRO	Peptide
16	X	96	VAL	Peptide
17	Y	33	ALA	Peptide
17	Y	36	SER	Peptide

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Mol	Chain	Res	Type	Group
30	Z	43	ASP	Peptide
30	Z	54	VAL	Peptide
30	Z	93	SER	Peptide
32	f	119	ARG	Peptide
32	f	138	ARG	Peptide
32	f	143	LYS	Peptide
32	f	147	VAL	Peptide
33	g	73	LEU	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	
2	A	204/252 (81%)	160 (78%)	42 (21%)	2 (1%)	15	52
3	B	111/255 (44%)	93 (84%)	15 (14%)	3 (3%)	5	35
4	C	215/254 (85%)	194 (90%)	20 (9%)	1 (0%)	29	66
5	E	258/261 (99%)	235 (91%)	22 (8%)	1 (0%)	34	70
6	G	224/236 (95%)	204 (91%)	15 (7%)	5 (2%)	6	39
7	H	182/190 (96%)	146 (80%)	29 (16%)	7 (4%)	3	29
8	I	184/200 (92%)	157 (85%)	25 (14%)	2 (1%)	14	51
9	J	183/197 (93%)	164 (90%)	17 (9%)	2 (1%)	14	51
10	L	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
11	N	148/151 (98%)	136 (92%)	9 (6%)	3 (2%)	7	41
12	O	16/137 (12%)	13 (81%)	3 (19%)	0	100	100
13	R	116/136 (85%)	103 (89%)	11 (10%)	2 (2%)	9	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	V	85/87 (98%)	64 (75%)	19 (22%)	2 (2%)	6	37
15	W	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
16	X	142/145 (98%)	115 (81%)	25 (18%)	2 (1%)	11	46
17	Y	132/135 (98%)	121 (92%)	11 (8%)	0	100	100
18	b	79/82 (96%)	66 (84%)	12 (15%)	1 (1%)	12	48
19	d	51/56 (91%)	48 (94%)	3 (6%)	0	100	100
20	e	58/63 (92%)	53 (91%)	5 (9%)	0	100	100
21	D	221/240 (92%)	203 (92%)	16 (7%)	2 (1%)	17	54
22	F	204/225 (91%)	177 (87%)	25 (12%)	2 (1%)	15	52
23	K	94/105 (90%)	76 (81%)	17 (18%)	1 (1%)	14	51
24	M	122/143 (85%)	88 (72%)	28 (23%)	6 (5%)	2	24
25	P	122/142 (86%)	101 (83%)	19 (16%)	2 (2%)	9	44
26	Q	139/143 (97%)	125 (90%)	11 (8%)	3 (2%)	6	39
27	S	143/146 (98%)	119 (83%)	21 (15%)	3 (2%)	7	40
28	T	141/144 (98%)	125 (89%)	16 (11%)	0	100	100
29	U	90/121 (74%)	83 (92%)	6 (7%)	1 (1%)	14	51
30	Z	68/108 (63%)	58 (85%)	9 (13%)	1 (2%)	10	46
31	c	61/67 (91%)	55 (90%)	6 (10%)	0	100	100
32	f	49/152 (32%)	37 (76%)	11 (22%)	1 (2%)	7	41
33	g	316/319 (99%)	285 (90%)	31 (10%)	0	100	100
All	All	4438/5178 (86%)	3854 (87%)	529 (12%)	55 (1%)	17	50

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	195	ILE
6	G	173	PRO
9	J	99	LEU
11	N	22	ALA
14	V	81	ASN
14	V	82	VAL
22	F	50	GLU
24	M	130	THR
24	M	131	ASP
26	Q	59	LYS

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Mol	Chain	Res	Type
27	S	91	ASP
3	B	180	THR
3	B	206	PRO
3	B	207	LEU
6	G	149	LYS
7	H	155	ASP
8	I	22	ARG
9	J	98	ALA
13	R	24	LEU
16	X	97	ASP
21	D	65	ARG
30	Z	44	GLN
2	A	4	PRO
2	A	196	SER
4	C	40	LYS
6	G	68	LEU
7	H	133	THR
13	R	86	PRO
24	M	126	TRP
25	P	12	PHE
25	P	125	PRO
26	Q	58	ASP
21	D	211	PRO
22	F	49	GLU
24	M	109	GLU
27	S	60	GLU
32	f	148	TYR
7	H	98	ILE
7	H	134	GLU
11	N	138	ASN
16	X	96	VAL
18	b	75	GLU
23	K	81	ASN
24	M	85	LYS
24	M	90	LYS
29	U	120	SER
6	G	67	VAL
6	G	174	LYS
27	S	92	ILE
7	H	65	PRO
8	I	152	ILE
7	H	132	PRO

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Mol	Chain	Res	Type
11	N	23	PRO
26	Q	33	GLY
7	H	131	PHE

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	A	164/210 (78%)	163 (99%)	1 (1%)	86	92
3	B	104/224 (46%)	104 (100%)	0	100	100
4	C	176/205 (86%)	175 (99%)	1 (1%)	86	92
5	E	221/222 (100%)	220 (100%)	1 (0%)	88	94
6	G	188/201 (94%)	185 (98%)	3 (2%)	62	79
7	H	165/170 (97%)	165 (100%)	0	100	100
8	I	150/161 (93%)	149 (99%)	1 (1%)	84	91
9	J	158/166 (95%)	154 (98%)	4 (2%)	47	70
10	L	129/137 (94%)	127 (98%)	2 (2%)	62	79
11	N	127/128 (99%)	126 (99%)	1 (1%)	81	89
12	O	15/105 (14%)	14 (93%)	1 (7%)	16	47
13	R	94/124 (76%)	93 (99%)	1 (1%)	73	85
14	V	74/74 (100%)	74 (100%)	0	100	100
15	W	110/111 (99%)	108 (98%)	2 (2%)	59	77
16	X	119/120 (99%)	119 (100%)	0	100	100
17	Y	112/113 (99%)	107 (96%)	5 (4%)	27	57
18	b	70/71 (99%)	70 (100%)	0	100	100
19	d	47/49 (96%)	43 (92%)	4 (8%)	10	40
20	e	51/54 (94%)	48 (94%)	3 (6%)	19	51
21	D	182/195 (93%)	176 (97%)	6 (3%)	38	65
22	F	173/191 (91%)	167 (96%)	6 (4%)	36	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	K	77/98 (79%)	76 (99%)	1 (1%)	69	82
24	M	88/119 (74%)	86 (98%)	2 (2%)	50	72
25	P	101/118 (86%)	100 (99%)	1 (1%)	76	86
26	Q	117/119 (98%)	116 (99%)	1 (1%)	78	88
27	S	128/129 (99%)	126 (98%)	2 (2%)	62	79
28	T	115/116 (99%)	111 (96%)	4 (4%)	36	64
29	U	93/114 (82%)	93 (100%)	0	100	100
30	Z	61/89 (68%)	59 (97%)	2 (3%)	38	65
31	c	56/60 (93%)	56 (100%)	0	100	100
32	f	43/135 (32%)	42 (98%)	1 (2%)	50	72
33	g	259/262 (99%)	255 (98%)	4 (2%)	65	81
All	All	3767/4390 (86%)	3707 (98%)	60 (2%)	64	79

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

Mol	Chain	Res	Type
2	A	185	ARG
4	C	119	LYS
5	E	240	LYS
6	G	68	LEU
6	G	98	ARG
6	G	170	THR
8	I	64	ASN
9	J	3	ARG
9	J	54	ARG
9	J	57	ARG
9	J	109	LEU
10	L	67	ARG
10	L	87	ARG
11	N	27	LYS
12	O	136	ARG
13	R	115	LEU
15	W	65	LEU
15	W	93	LEU
17	Y	32	ARG
17	Y	41	ARG
17	Y	102	LYS
17	Y	108	ARG

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Mol	Chain	Res	Type
17	Y	124	ARG
19	d	19	ARG
19	d	28	THR
19	d	46	LYS
19	d	48	ASN
20	e	26	LYS
20	e	33	ARG
20	e	53	LYS
21	D	4	LEU
21	D	67	ASN
21	D	76	ARG
21	D	111	ASN
21	D	178	ARG
21	D	190	ARG
22	F	25	LEU
22	F	69	PHE
22	F	122	ASN
22	F	157	ARG
22	F	194	LEU
22	F	225	ARG
23	K	40	LEU
24	M	43	ARG
24	M	125	ASN
25	P	36	LEU
26	Q	132	LYS
27	S	44	ASN
27	S	119	ILE
28	T	28	LEU
28	T	114	VAL
28	T	130	ARG
28	T	135	ILE
30	Z	42	LEU
30	Z	78	ILE
32	f	123	ASN
33	g	117	LYS
33	g	182	ASN
33	g	229	LYS
33	g	316	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	23	HIS
3	B	118	GLN
3	B	208	GLN
5	E	98	ASN
6	G	190	GLN
6	G	201	GLN
7	H	29	ASN
8	I	32	GLN
8	I	64	ASN
8	I	88	ASN
8	I	103	GLN
8	I	159	GLN
9	J	155	HIS
11	N	5	HIS
11	N	58	HIS
13	R	105	GLN
14	V	70	ASN
15	W	15	ASN
15	W	80	ASN
16	X	79	ASN
17	Y	63	GLN
17	Y	77	ASN
19	d	48	ASN
20	e	17	GLN
21	D	67	ASN
21	D	111	ASN
22	F	34	GLN
22	F	104	ASN
24	M	125	ASN
25	P	103	ASN
26	Q	32	ASN
27	S	71	GLN
27	S	78	HIS
28	T	43	ASN
30	Z	95	HIS
30	Z	98	GLN
31	c	51	ASN
32	f	123	ASN
33	g	182	ASN
33	g	195	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1743/1800 (96%)	625 (35%)	49 (2%)

All (625) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	14	C
1	2	20	G
1	2	23	G
1	2	24	U
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	42	G
1	2	43	A
1	2	45	U
1	2	46	A
1	2	47	A
1	2	50	C
1	2	57	G
1	2	60	U
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	100	A
1	2	104	A
1	2	105	A
1	2	114	C
1	2	115	G
1	2	126	A
1	2	127	G
1	2	128	U
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A

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Mol	Chain	Res	Type
1	2	136	C
1	2	137	U
1	2	138	A
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	176	C
1	2	178	U
1	2	179	A
1	2	183	U
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	201	G
1	2	202	A
1	2	212	U
1	2	215	A
1	2	218	A
1	2	219	A
1	2	223	U
1	2	226	A
1	2	229	U
1	2	231	U
1	2	233	C
1	2	234	G
1	2	236	A

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Mol	Chain	Res	Type
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	244	A
1	2	250	C
1	2	257	A
1	2	261	U
1	2	265	A
1	2	271	A
1	2	272	U
1	2	275	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	282	C
1	2	288	A
1	2	299	A
1	2	301	A
1	2	309	C
1	2	314	C
1	2	316	A
1	2	320	U
1	2	321	C
1	2	322	G
1	2	331	A
1	2	332	U
1	2	333	A
1	2	337	G
1	2	338	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	369	A
1	2	380	U
1	2	381	C
1	2	391	A
1	2	400	A
1	2	401	A

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Mol	Chain	Res	Type
1	2	402	C
1	2	404	G
1	2	416	A
1	2	417	A
1	2	418	G
1	2	419	G
1	2	421	A
1	2	424	C
1	2	425	A
1	2	426	G
1	2	434	G
1	2	435	C
1	2	439	U
1	2	444	C
1	2	448	C
1	2	452	A
1	2	453	U
1	2	454	U
1	2	464	A
1	2	468	A
1	2	469	C
1	2	475	A
1	2	477	A
1	2	478	A
1	2	481	A
1	2	484	C
1	2	485	A
1	2	486	G
1	2	487	G
1	2	490	C
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	501	U
1	2	502	U
1	2	504	U
1	2	505	A

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Mol	Chain	Res	Type
1	2	506	A
1	2	507	U
1	2	510	G
1	2	511	A
1	2	513	U
1	2	514	G
1	2	515	A
1	2	519	C
1	2	524	U
1	2	529	A
1	2	532	U
1	2	534	A
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	545	A
1	2	548	G
1	2	551	G
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	564	G
1	2	565	C
1	2	568	G
1	2	570	A
1	2	571	G
1	2	574	G
1	2	579	A
1	2	580	A
1	2	581	U
1	2	582	U
1	2	585	A
1	2	594	A
1	2	595	G
1	2	606	A
1	2	609	U

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Mol	Chain	Res	Type
1	2	611	U
1	2	619	A
1	2	620	A
1	2	621	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	634	G
1	2	635	A
1	2	639	U
1	2	648	G
1	2	649	U
1	2	650	U
1	2	652	G
1	2	653	C
1	2	654	C
1	2	655	G
1	2	656	G
1	2	658	C
1	2	677	G
1	2	679	U
1	2	680	U
1	2	684	A
1	2	685	A
1	2	686	C
1	2	687	G
1	2	691	C
1	2	694	U
1	2	695	U
1	2	696	C
1	2	697	C
1	2	698	U
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	712	G

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Mol	Chain	Res	Type
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	729	G
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	737	A
1	2	738	G
1	2	740	A
1	2	741	C
1	2	742	U
1	2	743	U
1	2	744	U
1	2	745	U
1	2	752	A
1	2	753	A
1	2	754	A
1	2	755	A
1	2	756	A
1	2	766	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	784	C
1	2	787	G
1	2	789	A
1	2	794	U

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Mol	Chain	Res	Type
1	2	795	U
1	2	803	A
1	2	807	A
1	2	808	U
1	2	811	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	818	C
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G
1	2	824	G
1	2	826	U
1	2	827	C
1	2	829	A
1	2	830	U
1	2	831	U
1	2	841	U
1	2	843	U
1	2	844	A
1	2	845	G
1	2	846	G
1	2	850	A
1	2	856	A
1	2	863	A
1	2	876	G
1	2	877	G
1	2	879	G
1	2	904	G
1	2	908	U
1	2	909	U
1	2	912	U
1	2	932	U
1	2	933	A
1	2	934	C
1	2	935	U
1	2	940	A
1	2	942	G
1	2	944	A

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Mol	Chain	Res	Type
1	2	953	G
1	2	960	U
1	2	961	U
1	2	966	A
1	2	973	A
1	2	977	A
1	2	990	C
1	2	992	A
1	2	993	A
1	2	996	U
1	2	997	G
1	2	998	A
1	2	1004	U
1	2	1005	A
1	2	1007	C
1	2	1011	G
1	2	1026	A
1	2	1028	C
1	2	1029	U
1	2	1030	A
1	2	1031	U
1	2	1032	G
1	2	1036	A
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1060	U
1	2	1061	A
1	2	1064	G
1	2	1072	C
1	2	1074	G
1	2	1075	C
1	2	1076	A
1	2	1078	C
1	2	1081	A
1	2	1082	C
1	2	1091	A
1	2	1092	A
1	2	1094	G
1	2	1096	C

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Mol	Chain	Res	Type
1	2	1097	U
1	2	1098	U
1	2	1100	G
1	2	1138	A
1	2	1143	A
1	2	1145	U
1	2	1147	A
1	2	1150	G
1	2	1151	A
1	2	1154	G
1	2	1155	G
1	2	1156	C
1	2	1158	C
1	2	1160	A
1	2	1161	C
1	2	1162	C
1	2	1163	A
1	2	1166	A
1	2	1167	G
1	2	1170	G
1	2	1171	A
1	2	1172	G
1	2	1174	C
1	2	1176	G
1	2	1185	U
1	2	1186	U
1	2	1191	U
1	2	1193	A
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1199	G
1	2	1200	G
1	2	1201	G
1	2	1202	A
1	2	1203	A
1	2	1207	C
1	2	1212	G
1	2	1213	G
1	2	1214	U
1	2	1217	A
1	2	1218	G

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Mol	Chain	Res	Type
1	2	1226	A
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1230	A
1	2	1233	G
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1247	U
1	2	1251	U
1	2	1254	U
1	2	1257	U
1	2	1258	U
1	2	1259	U
1	2	1260	U
1	2	1263	G
1	2	1265	G
1	2	1276	U
1	2	1284	C
1	2	1286	U
1	2	1297	G
1	2	1303	U
1	2	1305	U
1	2	1306	C
1	2	1312	A
1	2	1314	U
1	2	1315	U
1	2	1316	G
1	2	1319	A
1	2	1320	U
1	2	1321	A
1	2	1322	A
1	2	1323	C
1	2	1325	A
1	2	1327	C
1	2	1336	A
1	2	1337	A
1	2	1338	C
1	2	1339	C
1	2	1340	U
1	2	1341	A

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Mol	Chain	Res	Type
1	2	1344	A
1	2	1345	A
1	2	1347	U
1	2	1348	A
1	2	1349	G
1	2	1354	G
1	2	1355	C
1	2	1361	U
1	2	1363	U
1	2	1364	G
1	2	1367	G
1	2	1368	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1382	A
1	2	1385	G
1	2	1388	A
1	2	1390	U
1	2	1391	A
1	2	1392	U
1	2	1395	G
1	2	1396	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1412	G
1	2	1413	U
1	2	1415	U
1	2	1418	G
1	2	1421	A
1	2	1422	A
1	2	1423	U
1	2	1427	A
1	2	1428	G
1	2	1431	C
1	2	1432	U
1	2	1433	G
1	2	1437	U
1	2	1438	G
1	2	1439	C
1	2	1446	A

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Mol	Chain	Res	Type
1	2	1448	G
1	2	1456	C
1	2	1457	C
1	2	1458	G
1	2	1459	C
1	2	1464	G
1	2	1466	G
1	2	1469	A
1	2	1470	C
1	2	1473	U
1	2	1474	G
1	2	1475	A
1	2	1478	G
1	2	1479	A
1	2	1482	C
1	2	1486	G
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1496	U
1	2	1504	G
1	2	1506	G
1	2	1510	U
1	2	1515	A
1	2	1516	A
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1530	C
1	2	1531	G
1	2	1532	U
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1539	G
1	2	1540	G
1	2	1542	G
1	2	1543	A
1	2	1548	G
1	2	1557	U

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Mol	Chain	Res	Type
1	2	1559	A
1	2	1560	U
1	2	1561	U
1	2	1568	C
1	2	1569	A
1	2	1574	G
1	2	1577	A
1	2	1584	G
1	2	1593	A
1	2	1601	G
1	2	1611	A
1	2	1614	A
1	2	1616	G
1	2	1631	A
1	2	1632	C
1	2	1634	C
1	2	1635	A
1	2	1636	C
1	2	1637	C
1	2	1638	G
1	2	1640	C
1	2	1641	C
1	2	1649	G
1	2	1651	A
1	2	1652	C
1	2	1653	C
1	2	1654	G
1	2	1656	U
1	2	1657	U
1	2	1658	G
1	2	1659	A
1	2	1660	A
1	2	1661	U
1	2	1663	G
1	2	1665	U
1	2	1666	U
1	2	1680	G
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1712	A
1	2	1713	G

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Mol	Chain	Res	Type
1	2	1715	G
1	2	1716	C
1	2	1717	G
1	2	1731	A
1	2	1735	U
1	2	1736	G
1	2	1738	U
1	2	1739	C
1	2	1741	U
1	2	1742	U
1	2	1743	U
1	2	1744	A
1	2	1745	G
1	2	1748	G
1	2	1749	A
1	2	1750	A
1	2	1752	U
1	2	1753	A
1	2	1754	A
1	2	1755	A
1	2	1757	G
1	2	1758	U
1	2	1760	G
1	2	1761	U
1	2	1762	A
1	2	1763	A
1	2	1765	A
1	2	1766	A
1	2	1767	G
1	2	1769	U
1	2	1770	U
1	2	1771	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1790	A
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1796	C
1	2	1797	A

All (49) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	68	A
1	2	73	U
1	2	131	C
1	2	139	C
1	2	158	U
1	2	187	G
1	2	217	A
1	2	218	A
1	2	240	U
1	2	278	U
1	2	280	U
1	2	417	A
1	2	484	C
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	555	A
1	2	558	U
1	2	685	A
1	2	720	G
1	2	721	U
1	2	755	A
1	2	779	U
1	2	781	U
1	2	782	U
1	2	783	G
1	2	794	U
1	2	829	A
1	2	1051	G
1	2	1081	A
1	2	1196	A
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1296	A
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1568	C

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Mol	Chain	Res	Type
1	2	1573	A
1	2	1615	C
1	2	1630	U
1	2	1650	U
1	2	1652	C
1	2	1734	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
1	2	2
29	U	2
4	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	839:U	O3'	840:U	P	4.31
1	2	1654:G	O3'	1655:A	P	4.14
1	U	84:MET	C	85:ARG	N	3.97
1	U	61:LYS	C	62:VAL	N	3.80

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	225:LEU	C	226:THR	N	1.20

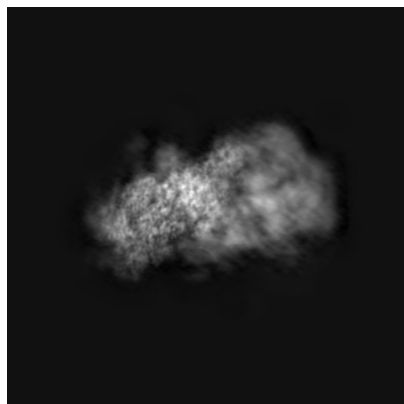
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4793. These allow visual inspection of the internal detail of the map and identification of artifacts.

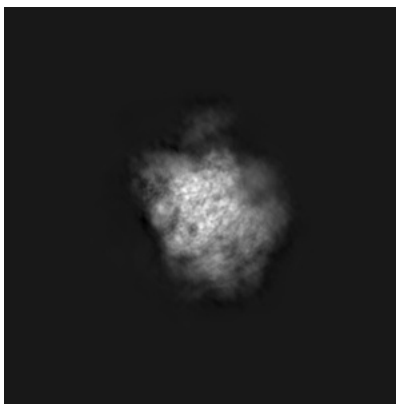
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

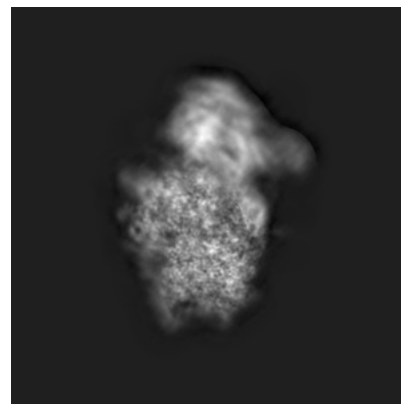
6.1.1 Primary map



X

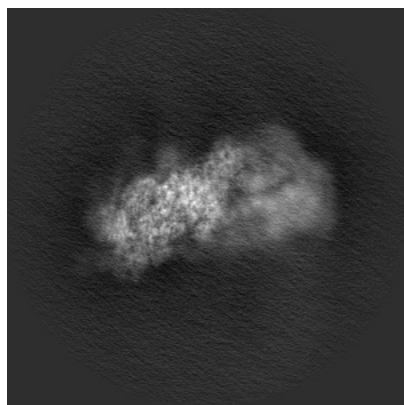


Y

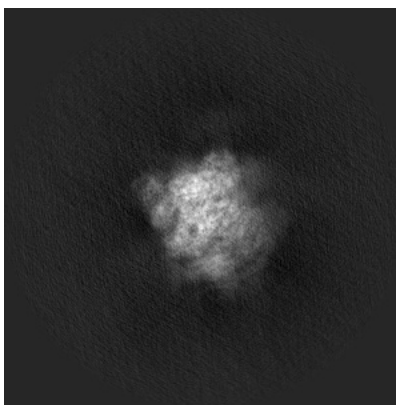


Z

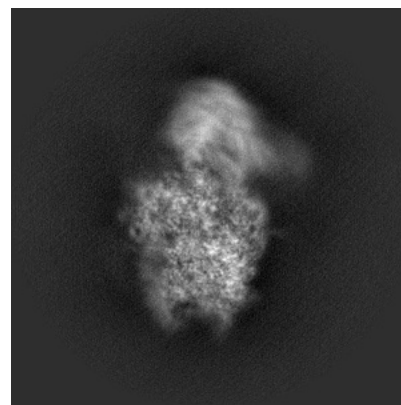
6.1.2 Raw map



X



Y

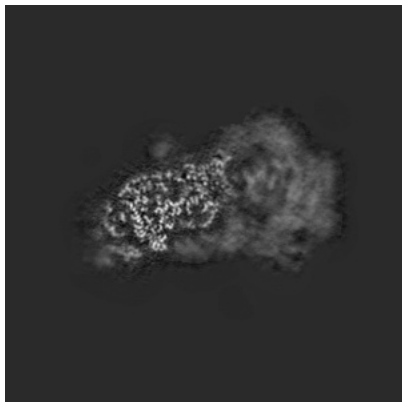


Z

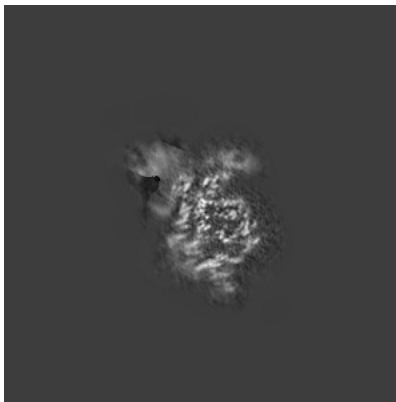
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

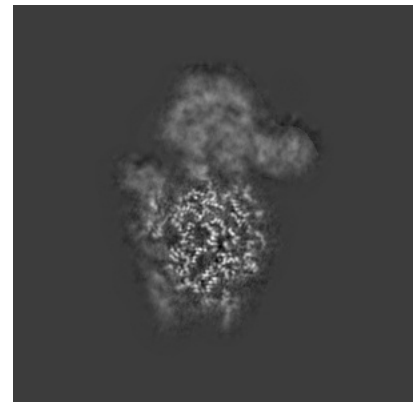
6.2.1 Primary map



X Index: 192

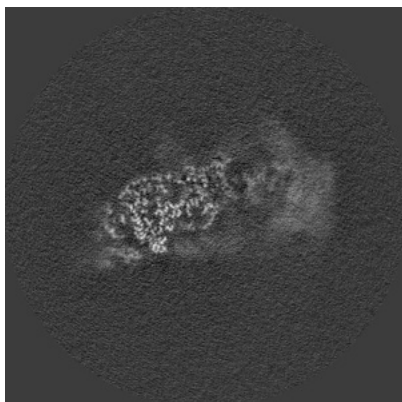


Y Index: 192

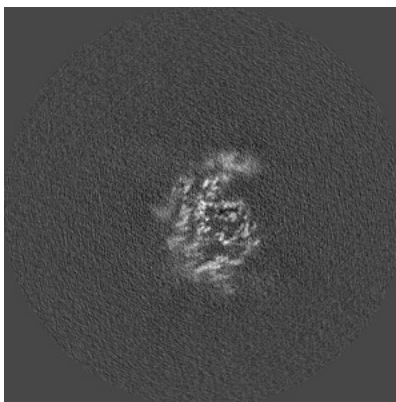


Z Index: 192

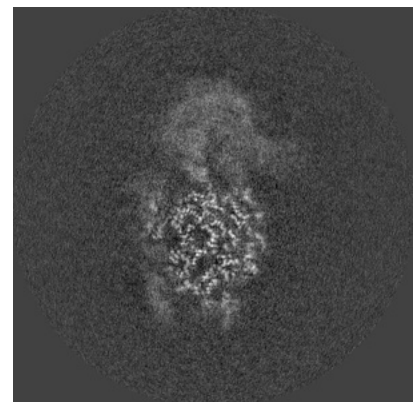
6.2.2 Raw map



X Index: 192



Y Index: 192

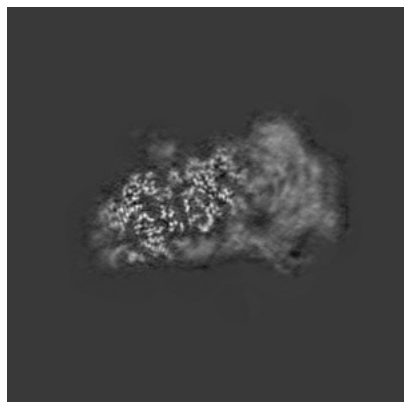


Z Index: 192

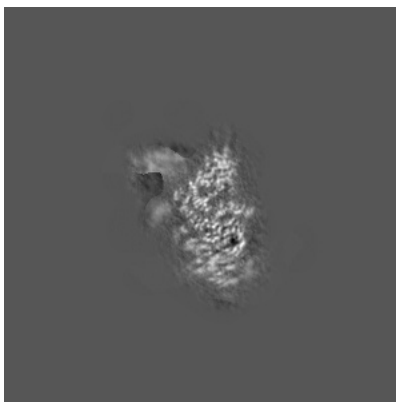
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

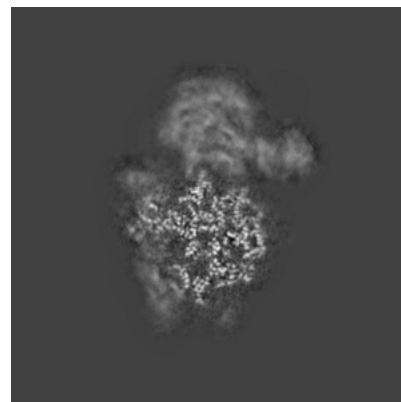
6.3.1 Primary map



X Index: 185

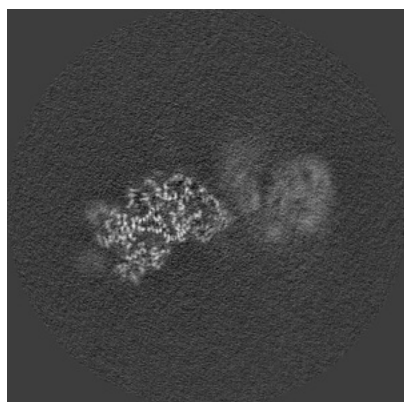


Y Index: 177

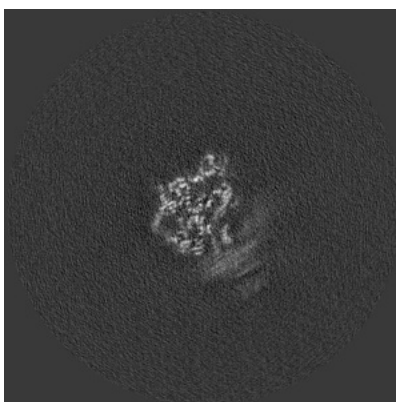


Z Index: 197

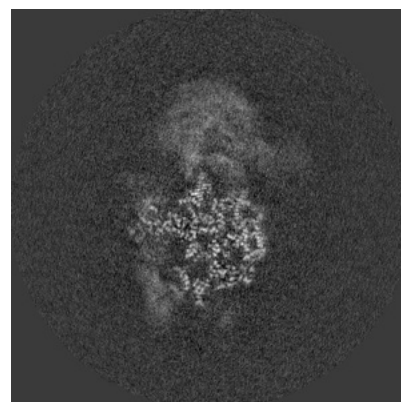
6.3.2 Raw map



X Index: 208



Y Index: 152

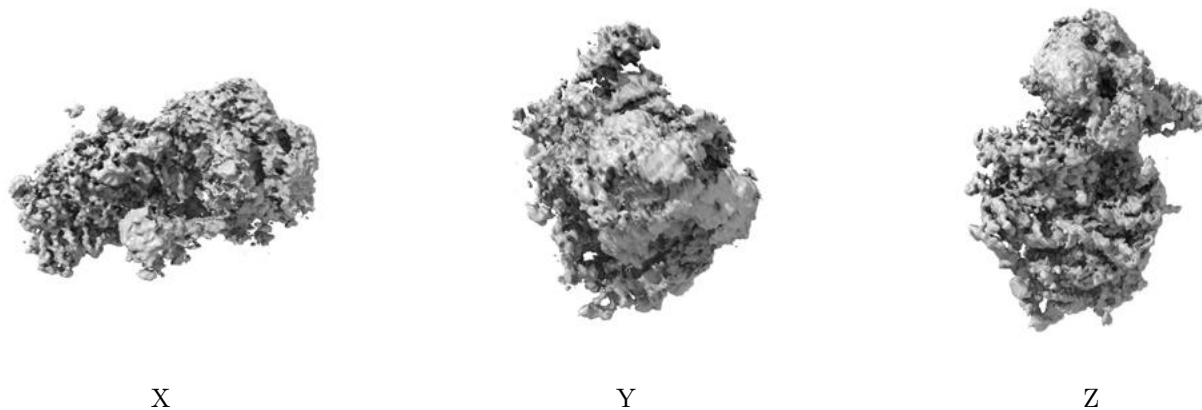


Z Index: 197

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

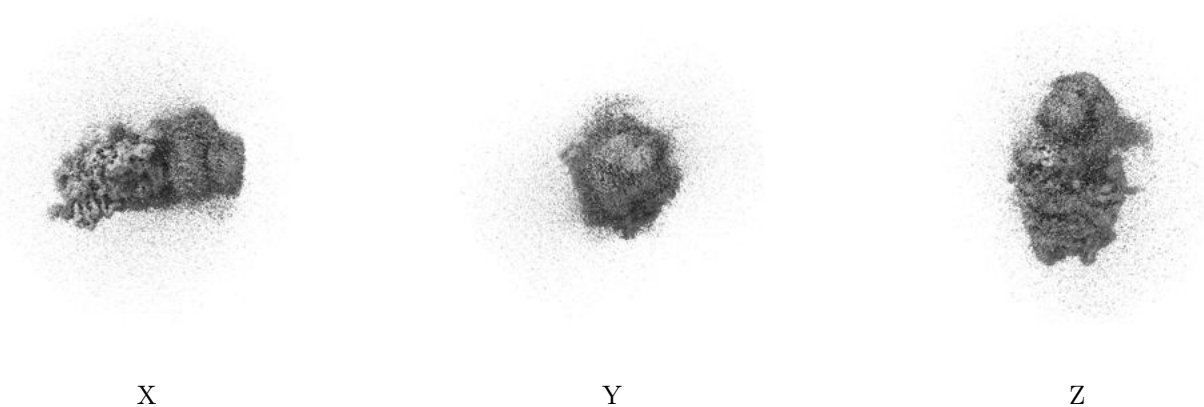
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

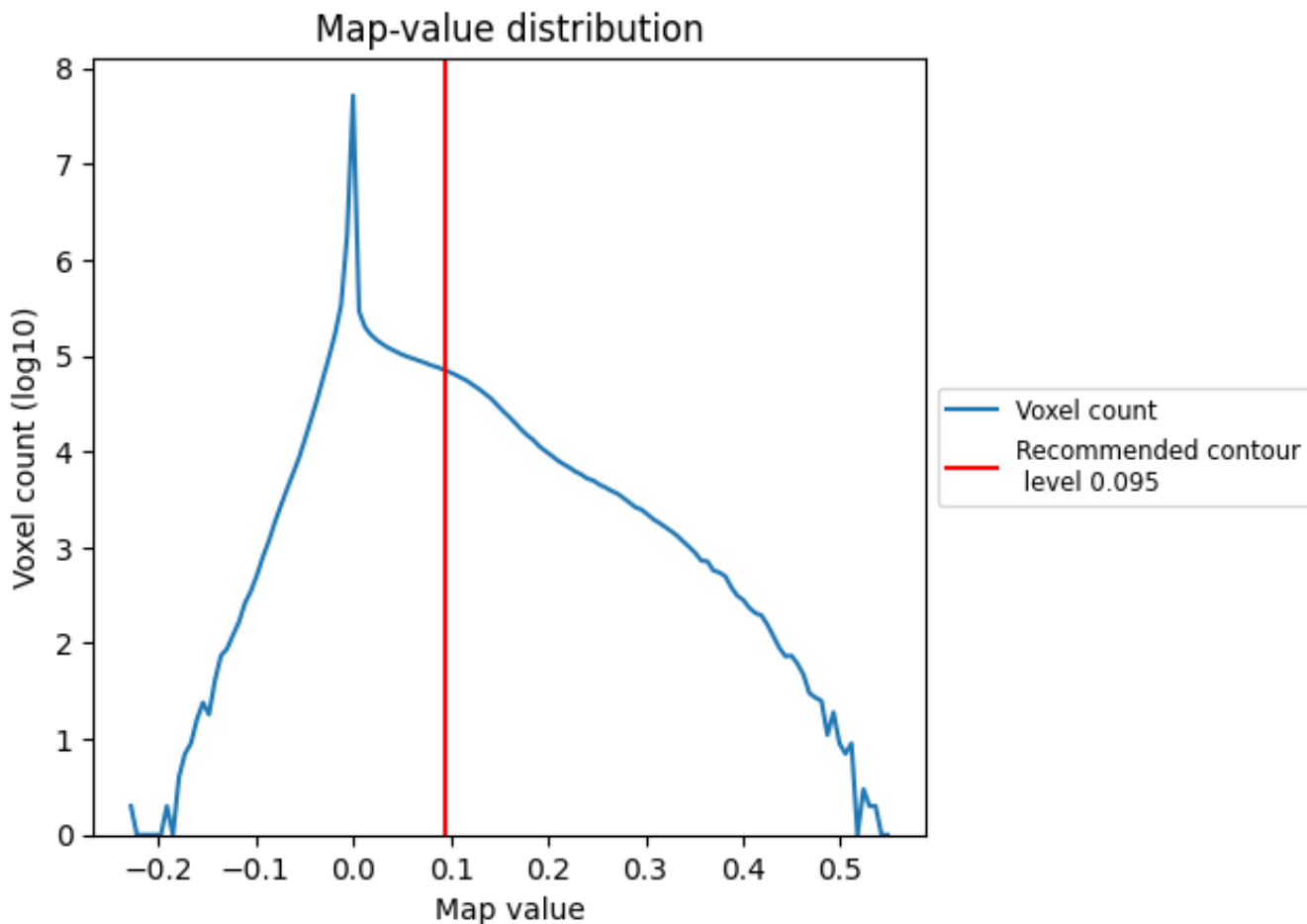
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

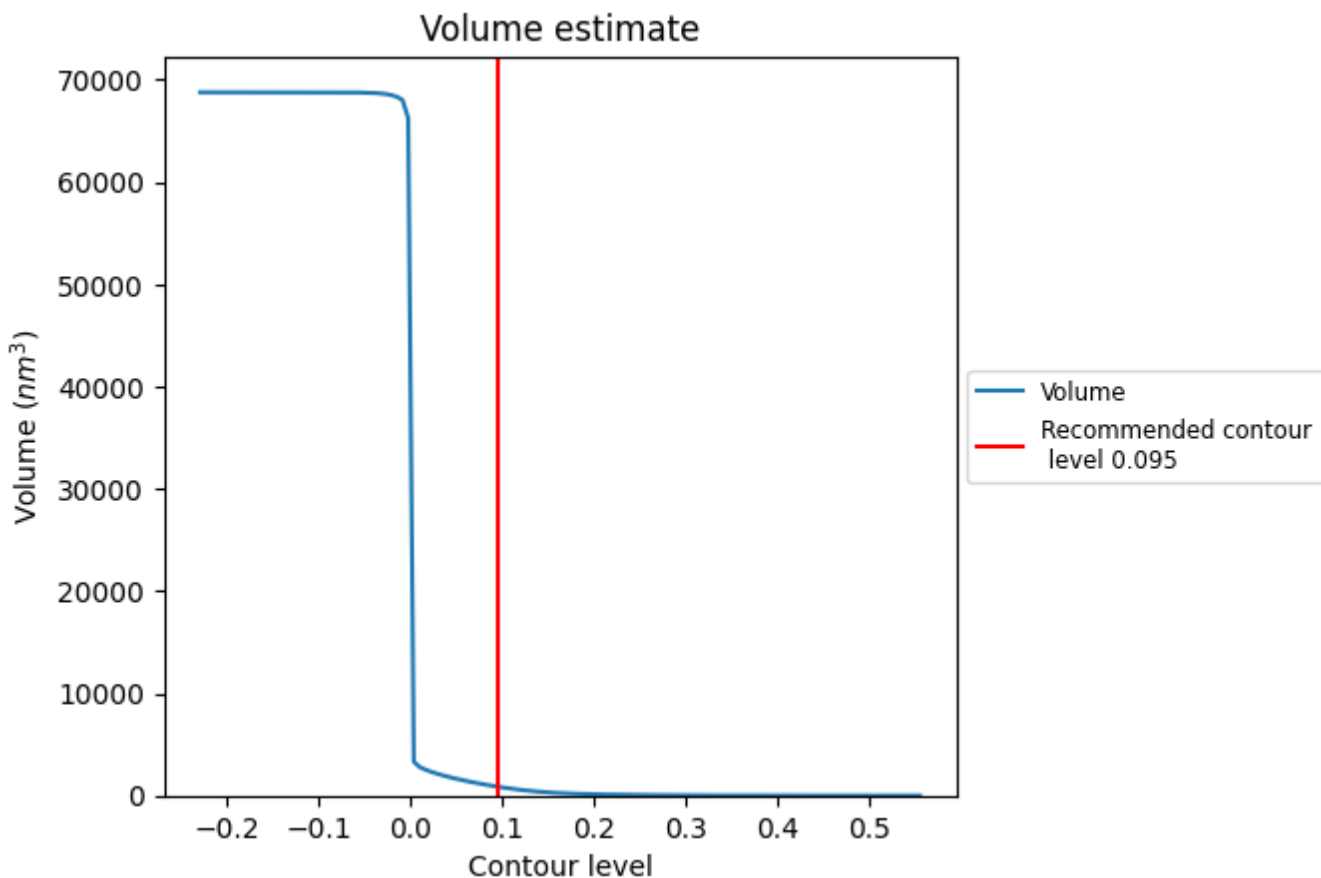
This section contains the results of statistical analysis of the map.

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.

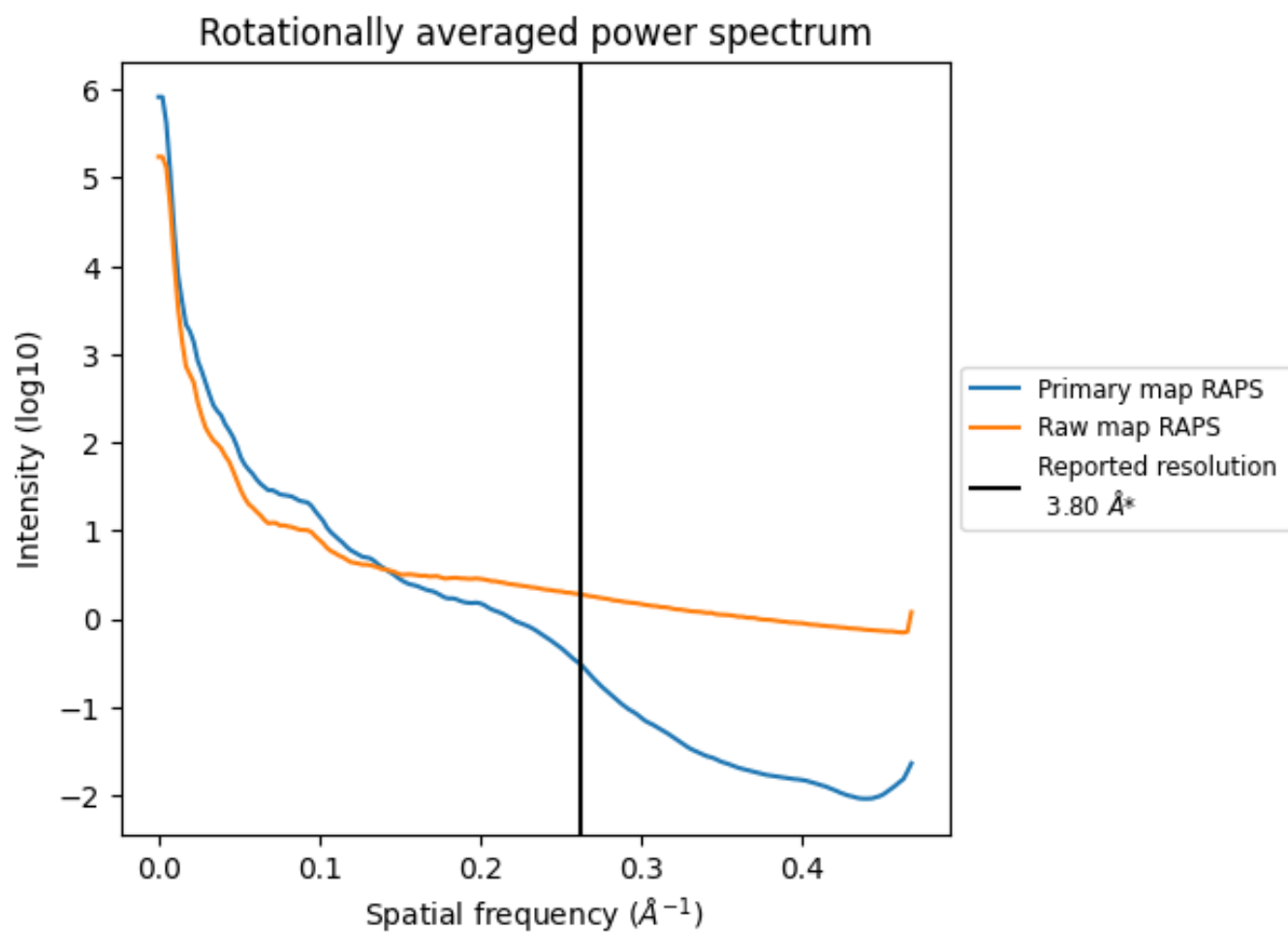
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 871 nm³; this corresponds to an approximate mass of 787 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

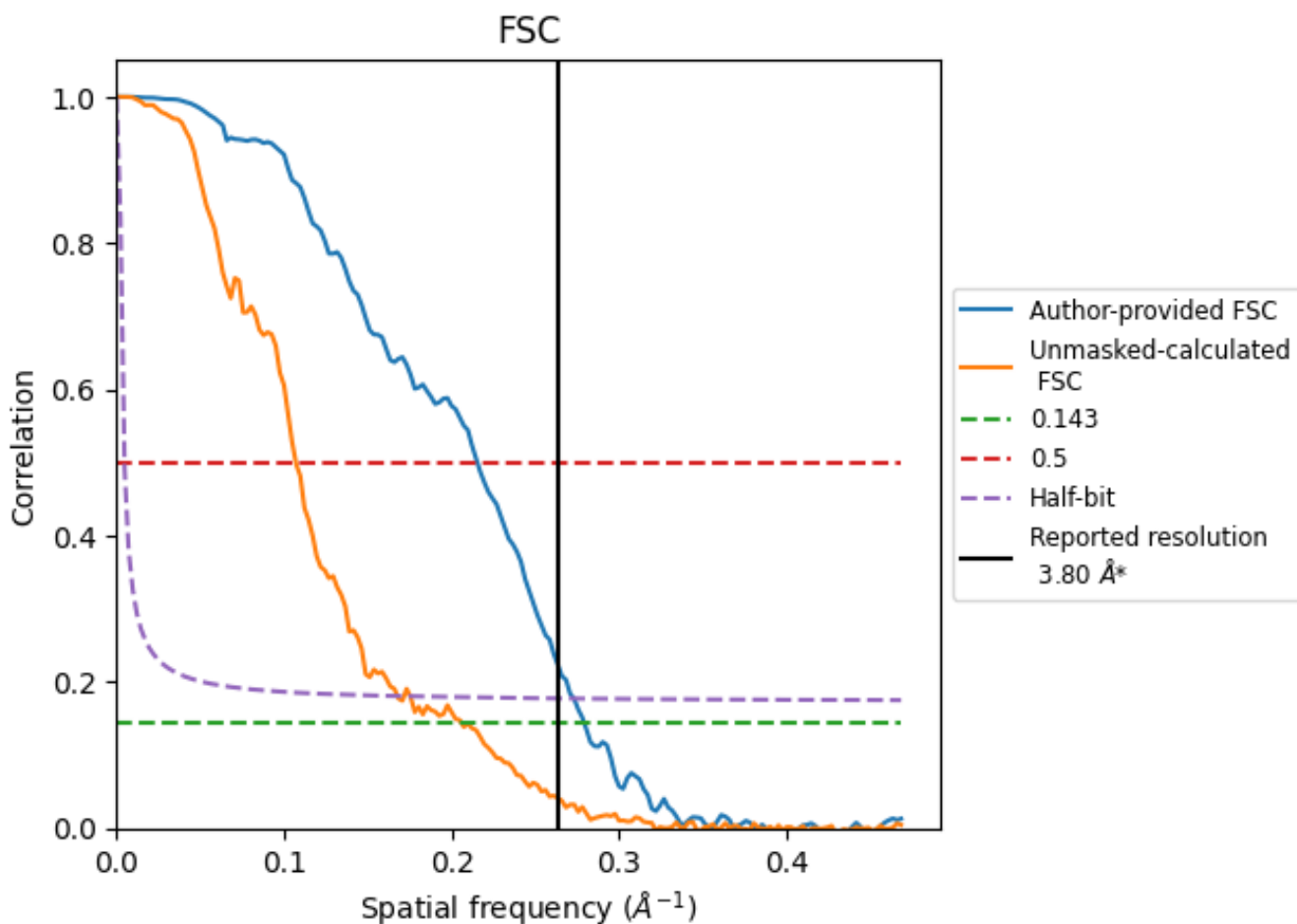


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

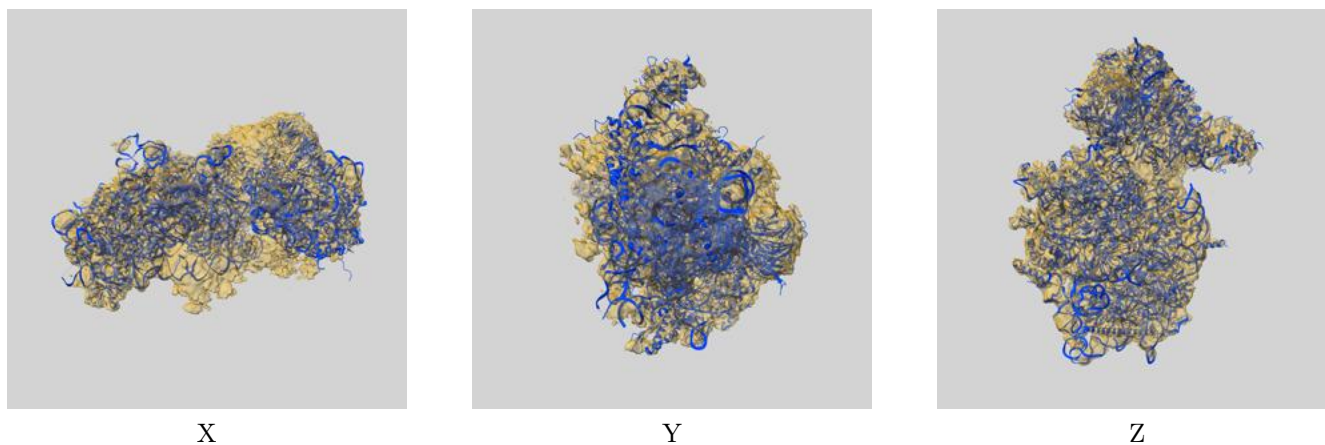
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.58	4.64	3.66
Unmasked-calculated*	4.85	9.33	5.96

*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 4.85 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4793 and PDB model 6RBE. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



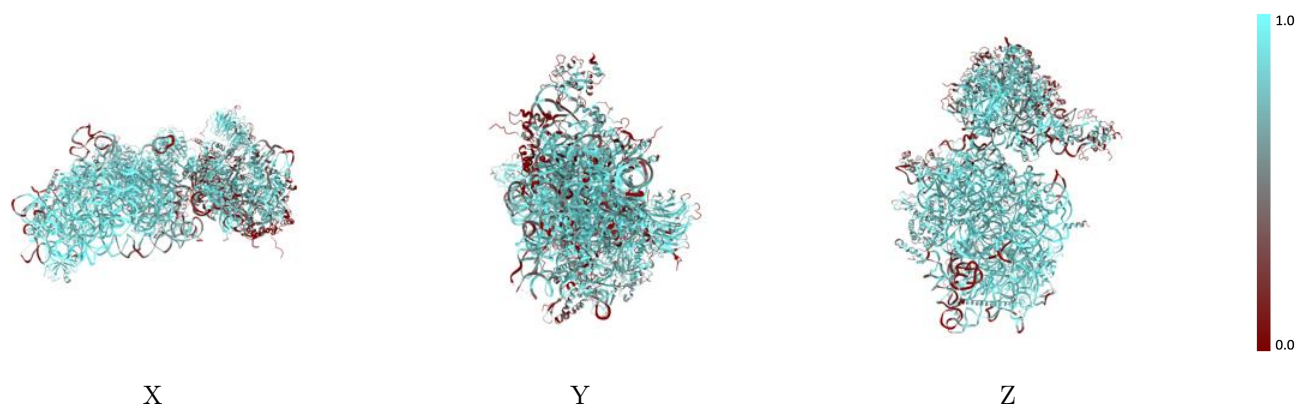
The images above show the 3D surface view of the map at the recommended contour level 0.095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



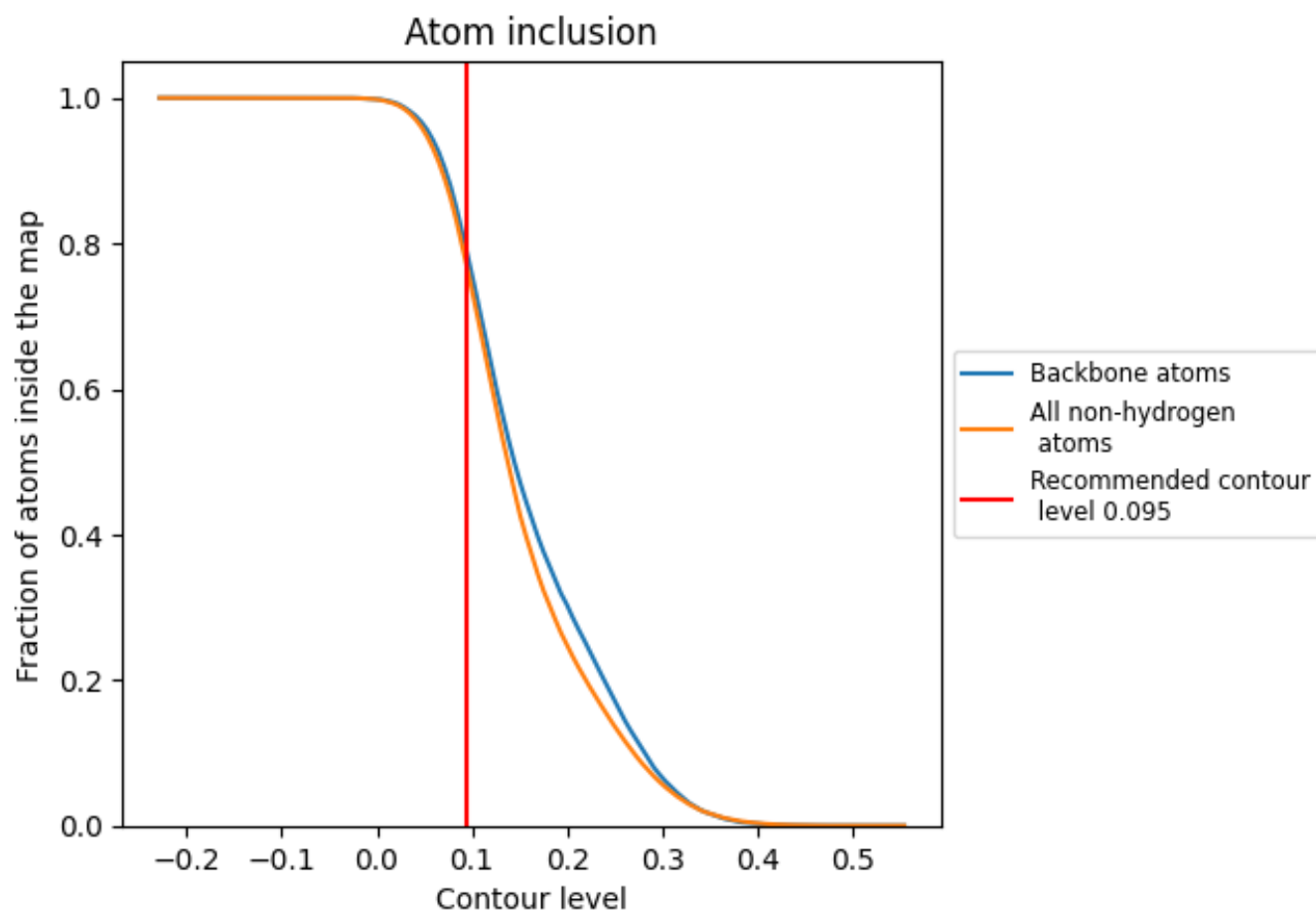
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.095).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 77% 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 (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7670	 0.2780
2	 0.7992	 0.2930
A	 0.9086	 0.3990
B	 0.3826	 0.1560
C	 0.9030	 0.4240
D	 0.6655	 0.1310
E	 0.9290	 0.4810
F	 0.6849	 0.0870
G	 0.8540	 0.4230
H	 0.7011	 0.2560
I	 0.8788	 0.4380
J	 0.8717	 0.4030
K	 0.7559	 0.1140
L	 0.8528	 0.4560
M	 0.4489	 0.0970
N	 0.7792	 0.2970
O	 0.2519	 0.0740
P	 0.3888	 0.0740
Q	 0.6664	 0.0600
R	 0.6200	 0.1720
S	 0.2877	 0.0570
T	 0.7114	 0.0740
U	 0.6023	 0.1250
V	 0.8976	 0.3880
W	 0.9269	 0.4450
X	 0.8857	 0.4230
Y	 0.8790	 0.4440
Z	 0.4607	 0.0800
b	 0.7637	 0.3250
c	 0.4822	 0.1040
d	 0.5863	 0.0830
e	 0.6688	 0.3480
f	 0.3152	 0.0710
g	 0.7691	 0.0970

