



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:50 AM EST

PDB ID : 3J0P
EMDB ID : EMD-5328
Title : Core of mammalian 80S pre-ribosome in complex with tRNAs fitted to a 10.6Å cryo-em map: rotated PRE state 1
Authors : Budkevich, T.; Giesebrecht, J.; Altman, R.; Munro, J.; Mielke, T.; Nierhaus, K.; Blanchard, S.; Spahn, C.M.
Deposited on : 2011-10-06
Resolution : 10.60 Å(reported)
Based on initial models : 2XZM, 3O58

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

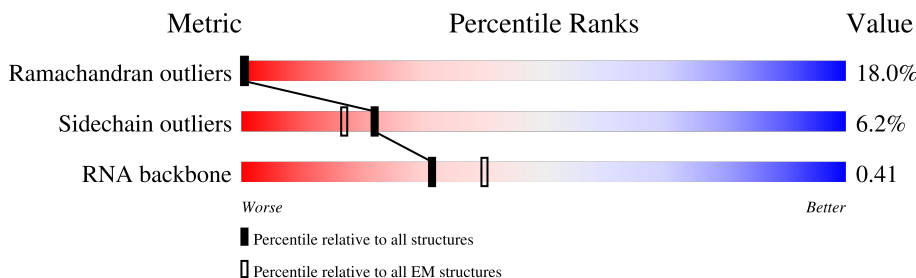
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.60 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.











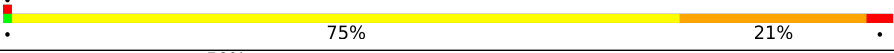

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	48	<div> <div>65%</div> <div>25%</div> <div>6%</div> <div>.</div> </div>
2	c	17	<div> <div>71%</div> <div>29%</div> </div>
3	d	7	<div> <div>71%</div> <div>14%</div> <div>14%</div> </div>
4	g	31	<div> <div>71%</div> <div>23%</div> <div>6%</div> </div>
5	G	13	<div> <div>85%</div> <div>15%</div> </div>
6	f	21	<div> <div>76%</div> <div>24%</div> </div>
7	h	111	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
8	S	125	<div> <div>6%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	L	141	 82% 17% .
10	X	68	 21% 88% 12%
11	2	112	 38% 50% 12% .
12	3	12	 8% 50% 50%
13	7	50	 28% 56% 16%
14	B	213	 16% 67% 30% .
15	Y	75	 5% 72% 28%
16	y	3	 100%
17	W	77	 75% 21% .
18	w	2	 50% 100%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 16039 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 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	48	Total	C	N	O	P	0	0
			1029	459	190	332	48		

- Molecule 2 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	17	Total	C	N	O	P	0	0
			362	162	66	117	17		

- Molecule 3 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	7	Total	C	N	O	P	0	0
			155	69	33	46	7		

- Molecule 4 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	31	Total	C	N	O	P	0	0
			660	295	118	216	31		

- Molecule 5 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	13	Total	C	N	O	P	0	0
			276	123	49	91	13		

- Molecule 6 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	21	Total	C	N	O	P	0	0
			452	200	79	152	21		

- Molecule 7 is a RNA chain called 40S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	111	Total	C	N	O	P	0	0
			2368	1060	431	766	111		

- Molecule 8 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	125	Total	C	N	O	S	0	0
			985	632	173	176	4		

- Molecule 9 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	141	Total	C	N	O	S	0	0
			1097	691	221	180	5		

- Molecule 10 is a protein called Ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	68	Total	C	N	O	S	0	0
			554	350	113	90	1		

- Molecule 11 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	112	Total	C	N	O	P	0	0
			2392	1070	435	775	112		

- Molecule 12 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	12	Total	C	N	O	P	0	0
			259	116	50	81	12		

- Molecule 13 is a RNA chain called 60S ribosomal RNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	7	50	Total	C	N	O	P	0	0
			1054	471	173	360	50		

- Molecule 14 is a protein called Ribosomal protein L10a.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	B	213	Total	C	N	O	0	0
			1055	629	213	213		

- Molecule 15 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	75	Total	C	N	O	P	0	0
			1597	713	285	525	74		

- Molecule 16 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	y	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

- Molecule 17 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

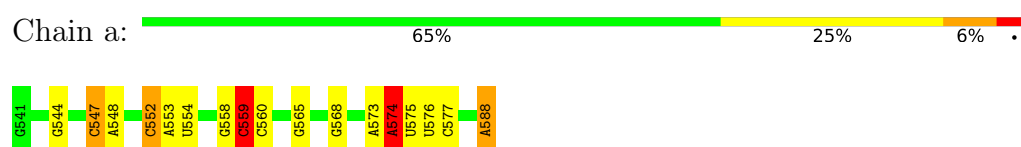
- Molecule 18 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	w	2	Total	C	N	O	P	0	0
			44	20	10	12	2		

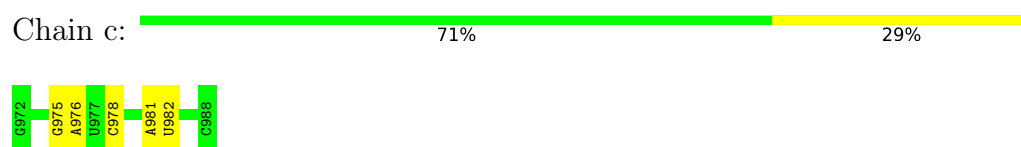
3 Residue-property plots [i](#)

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.

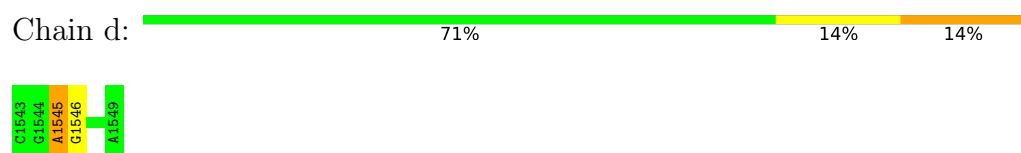
- Molecule 1: 40S ribosomal RNA fragment



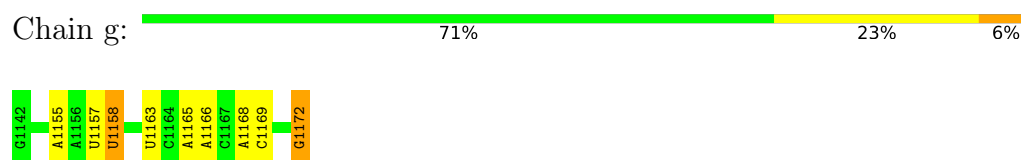
- Molecule 2: 40S ribosomal RNA fragment



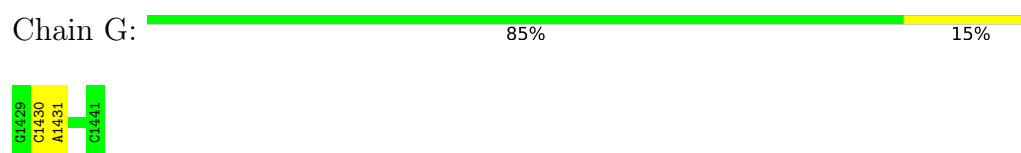
- Molecule 3: 40S ribosomal RNA fragment



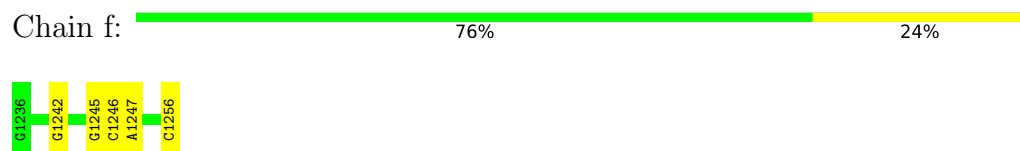
- Molecule 4: 40S ribosomal RNA fragment



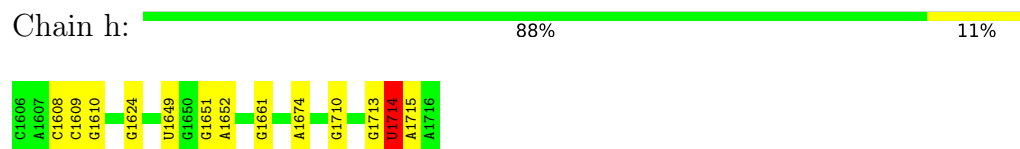
- Molecule 5: 40S ribosomal RNA fragment



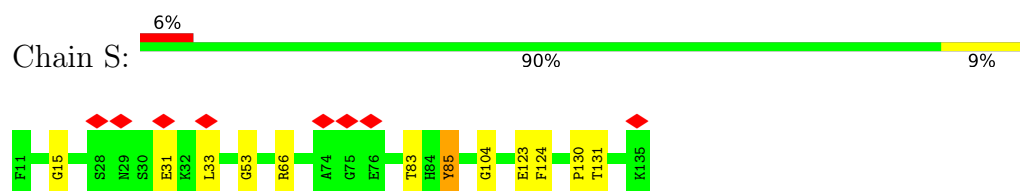
- Molecule 6: 40S ribosomal RNA fragment



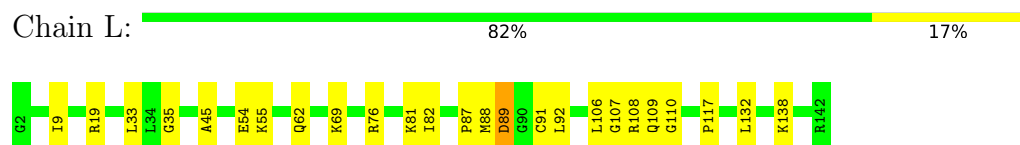
- Molecule 7: 40S ribosomal RNA fragment



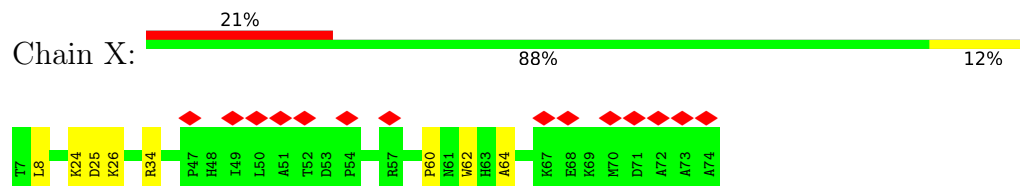
- Molecule 8: Ribosomal protein S15



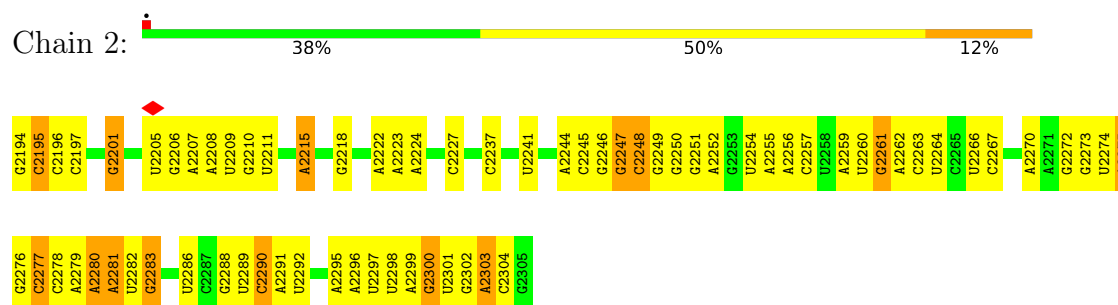
- Molecule 9: Ribosomal protein S23



- Molecule 10: Ribosomal protein S30

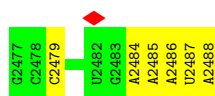


- Molecule 11: 60S ribosomal RNA fragment



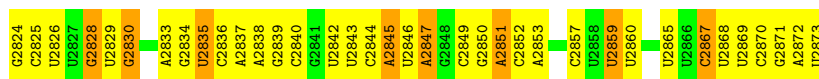
- Molecule 12: 60S ribosomal RNA fragment





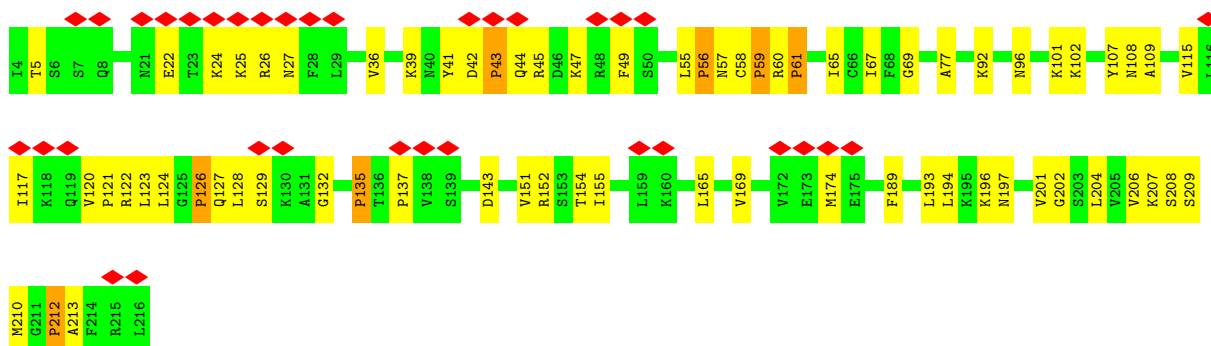
- Molecule 13: 60S ribosomal RNA fragment

Chain 7: 28% 56% 16%



- Molecule 14: Ribosomal protein L10a

Chain B: 16% 67% 30%



- Molecule 15: tRNA

Chain Y: 5% 72% 28%



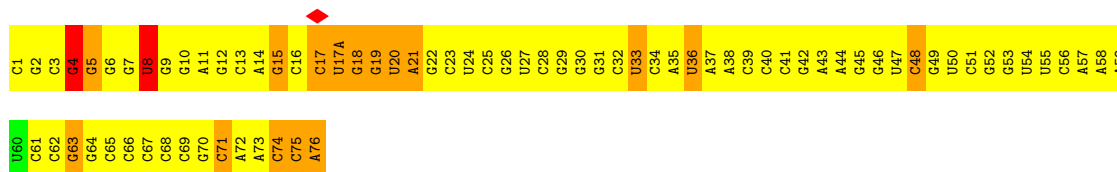
- Molecule 16: mRNA fragment

Chain y: 100%

There are no outlier residues recorded for this chain.

- Molecule 17: tRNA

Chain W: 75% 21%



- Molecule 18: mRNA fragment



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22212	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF CORRECTION OF EACH DEFOCUS GROUP VOLUME PRIOR TO BACK PROJECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	65520	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	17178.881	Depositor
Minimum map value	-2915.682	Depositor
Average map value	268.573	Depositor
Map value standard deviation	1207.565	Depositor
Recommended contour level	1000.0	Depositor
Map size (\AA)	453.6, 453.6, 453.6	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.52, 2.52, 2.52	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	a	0.69	2/1151 (0.2%)	0.99	8/1793 (0.4%)
2	c	0.64	0/404	0.91	1/627 (0.2%)
3	d	0.49	0/174	0.84	0/270
4	g	0.60	0/737	0.87	2/1146 (0.2%)
5	G	0.52	0/307	0.82	0/476
6	f	0.58	0/504	0.87	0/785
7	h	0.45	0/2650	0.74	1/4127 (0.0%)
8	S	0.39	0/1003	0.66	1/1342 (0.1%)
9	L	0.43	0/1114	0.74	0/1485
10	X	0.35	0/566	0.71	0/753
11	2	1.10	4/2677 (0.1%)	1.68	69/4170 (1.7%)
12	3	0.18	0/290	0.43	0/450
13	7	1.07	2/1174 (0.2%)	2.34	33/1825 (1.8%)
14	B	0.34	0/1054	0.63	9/1468 (0.6%)
15	Y	0.47	0/1784	0.74	0/2780
16	y	0.39	0/65	0.69	0/98
17	W	2.74	133/1832 (7.3%)	2.53	181/2855 (6.3%)
18	w	0.40	0/49	0.79	0/74
All	All	1.10	141/17535 (0.8%)	1.38	305/26524 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	3
3	d	0	1
4	g	0	2
7	h	0	2
17	W	0	5
All	All	0	13

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	W	59	A	N9-C4	-13.33	1.29	1.37
17	W	2	G	C8-N7	-13.19	1.23	1.30
17	W	40	C	N1-C6	-12.02	1.29	1.37
13	7	2845	A	C6-N1	-10.99	1.27	1.35
17	W	22	G	N7-C5	-10.51	1.32	1.39
17	W	72	A	N9-C4	-10.01	1.31	1.37
17	W	49	G	N9-C8	-9.55	1.31	1.37
17	W	24	U	C4-O4	-9.29	1.16	1.23
17	W	49	G	N7-C5	-9.12	1.33	1.39
17	W	16	C	N1-C6	-9.12	1.31	1.37
17	W	57	A	N7-C5	-8.89	1.33	1.39
17	W	10	G	C5-C6	-8.69	1.33	1.42
17	W	30	G	C2'-C1'	-8.65	1.43	1.53
17	W	48	C	C2-N3	-8.59	1.28	1.35
17	W	9	G	N7-C5	-8.52	1.34	1.39
17	W	51	C	C2-N3	-8.24	1.29	1.35
17	W	21	A	N9-C4	-8.23	1.32	1.37
17	W	27	U	C2-N3	-8.12	1.32	1.37
17	W	61	C	C5-C6	-7.96	1.27	1.34
17	W	3	C	N3-C4	-7.91	1.28	1.33
17	W	31	G	C8-N7	-7.74	1.26	1.30
17	W	15	G	C6-N1	-7.74	1.34	1.39
17	W	62	C	C4-C5	-7.59	1.36	1.43
17	W	33	U	C2-N3	-7.58	1.32	1.37
17	W	39	C	C4-N4	-7.57	1.27	1.33
17	W	65	C	C4-C5	-7.49	1.36	1.43
17	W	57	A	N9-C4	-7.45	1.33	1.37
17	W	58	A	N3-C4	-7.45	1.30	1.34
17	W	69	C	C2-N3	-7.42	1.29	1.35
17	W	35	A	N7-C5	-7.41	1.34	1.39
17	W	36	U	C3'-C2'	-7.40	1.44	1.52
17	W	73	A	C5-C4	-7.30	1.33	1.38
17	W	67	C	P-O5'	-7.23	1.52	1.59
17	W	71	C	N1-C2	-7.22	1.32	1.40
17	W	53	G	N7-C5	-7.15	1.34	1.39
17	W	39	C	N1-C6	-7.13	1.32	1.37
17	W	69	C	N3-C4	7.10	1.39	1.33
17	W	38	A	C8-N7	-7.09	1.26	1.31
17	W	22	G	C4'-C3'	-7.04	1.45	1.53
17	W	43	A	N3-C4	-6.99	1.30	1.34
17	W	30	G	C6-O6	-6.97	1.17	1.24
17	W	19	G	C2-N3	-6.96	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	W	10	G	P-O5'	-6.88	1.52	1.59
17	W	45	G	N9-C4	-6.82	1.32	1.38
17	W	18	G	N9-C4	-6.81	1.32	1.38
17	W	30	G	N3-C4	-6.79	1.30	1.35
17	W	63	G	C5-C6	-6.75	1.35	1.42
17	W	7	G	P-O5'	-6.64	1.53	1.59
17	W	32	C	N3-C4	-6.64	1.29	1.33
17	W	34	C	N1-C6	-6.61	1.33	1.37
17	W	58	A	P-O5'	-6.60	1.53	1.59
17	W	17	C	C2'-C1'	-6.56	1.46	1.53
17	W	17(A)	U	C2-N3	-6.55	1.33	1.37
17	W	25	C	C2-O2	-6.53	1.18	1.24
17	W	59	A	C8-N7	-6.50	1.27	1.31
17	W	12	G	N7-C5	-6.49	1.35	1.39
17	W	72	A	N9-C8	-6.47	1.32	1.37
17	W	16	C	C4-C5	6.45	1.48	1.43
17	W	12	G	C8-N7	-6.43	1.27	1.30
17	W	41	C	C2-O2	-6.42	1.18	1.24
17	W	8	U	C4-C5	-6.42	1.37	1.43
17	W	18	G	C3'-C2'	-6.42	1.45	1.52
17	W	64	G	C6-N1	-6.41	1.35	1.39
17	W	5	G	C8-N7	-6.36	1.27	1.30
17	W	56	C	C4'-C3'	-6.36	1.46	1.53
17	W	8	U	C2-O2	-6.33	1.16	1.22
17	W	12	G	N3-C4	-6.29	1.31	1.35
17	W	18	G	C5-C4	-6.29	1.33	1.38
17	W	32	C	C3'-C2'	-6.26	1.45	1.52
17	W	41	C	C4-N4	-6.23	1.28	1.33
17	W	44	A	C5-C4	-6.18	1.34	1.38
11	2	2283	G	N9-C8	6.17	1.42	1.37
17	W	33	U	C4'-C3'	-6.16	1.46	1.53
17	W	3	C	C4-C5	-6.16	1.38	1.43
17	W	34	C	C4-C5	-6.10	1.38	1.43
17	W	72	A	N7-C5	-6.02	1.35	1.39
17	W	14	A	C6-N1	-6.01	1.31	1.35
17	W	73	A	C8-N7	-5.95	1.27	1.31
17	W	63	G	P-O5'	-5.92	1.53	1.59
17	W	44	A	C8-N7	-5.92	1.27	1.31
17	W	11	A	N1-C2	-5.91	1.29	1.34
17	W	3	C	C3'-C2'	-5.90	1.46	1.52
17	W	14	A	P-O5'	-5.89	1.53	1.59
17	W	42	G	C8-N7	-5.89	1.27	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	W	36	U	C2-O2	-5.88	1.17	1.22
17	W	63	G	C8-N7	-5.87	1.27	1.30
17	W	76	A	C8-N7	-5.85	1.27	1.31
17	W	9	G	C8-N7	-5.84	1.27	1.30
17	W	11	A	P-O5'	-5.82	1.53	1.59
17	W	71	C	C4-C5	-5.79	1.38	1.43
17	W	46	G	N1-C2	-5.79	1.33	1.37
17	W	11	A	O4'-C1'	-5.78	1.34	1.41
17	W	36	U	P-O5'	-5.76	1.53	1.59
17	W	58	A	N9-C8	-5.75	1.33	1.37
17	W	43	A	N7-C5	-5.74	1.35	1.39
17	W	21	A	C2-N3	-5.72	1.28	1.33
17	W	58	A	N1-C2	-5.68	1.29	1.34
17	W	25	C	C4'-C3'	-5.67	1.46	1.52
17	W	21	A	C5-C6	-5.65	1.35	1.41
17	W	30	G	C4'-C3'	-5.59	1.47	1.52
17	W	45	G	C6-N1	-5.55	1.35	1.39
17	W	45	G	C1'-N9	-5.52	1.39	1.46
17	W	70	G	C8-N7	-5.50	1.27	1.30
17	W	9	G	N9-C8	-5.48	1.34	1.37
17	W	55	U	C5-C6	-5.44	1.29	1.34
17	W	28	C	C4'-C3'	-5.43	1.47	1.52
1	a	565	G	N9-C4	5.41	1.42	1.38
17	W	17(A)	U	C2-O2	-5.39	1.17	1.22
17	W	27	U	C4'-C3'	5.38	1.59	1.53
17	W	56	C	N3-C4	-5.36	1.30	1.33
17	W	57	A	N9-C8	-5.35	1.33	1.37
17	W	56	C	C5-C6	-5.34	1.30	1.34
17	W	62	C	C4'-C3'	-5.34	1.47	1.52
17	W	64	G	C8-N7	-5.34	1.27	1.30
17	W	61	C	C4'-C3'	-5.34	1.47	1.52
17	W	43	A	C5-C6	-5.31	1.36	1.41
17	W	11	A	C8-N7	-5.29	1.27	1.31
17	W	45	G	N3-C4	-5.28	1.31	1.35
17	W	46	G	C3'-C2'	-5.28	1.47	1.52
17	W	32	C	N1-C2	-5.24	1.34	1.40
17	W	74	C	C4'-O4'	-5.24	1.38	1.45
17	W	14	A	C1'-N9	-5.21	1.39	1.46
17	W	73	A	N1-C2	-5.21	1.29	1.34
17	W	22	G	C3'-C2'	-5.21	1.47	1.52
17	W	50	U	N3-C4	-5.18	1.33	1.38
11	2	2302	G	C6-N1	-5.17	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	W	23	C	C4'-C3'	-5.17	1.47	1.52
17	W	53	G	C2-N3	-5.13	1.28	1.32
17	W	59	A	C6-N6	-5.12	1.29	1.33
11	2	2279	A	N7-C5	-5.12	1.36	1.39
17	W	46	G	N9-C4	-5.10	1.33	1.38
17	W	19	G	C6-O6	-5.09	1.19	1.24
17	W	18	G	N9-C8	5.06	1.41	1.37
17	W	22	G	N9-C8	-5.05	1.34	1.37
17	W	37	A	C2-N3	-5.05	1.29	1.33
13	7	2830	G	N3-C4	-5.02	1.31	1.35
17	W	49	G	N3-C4	-5.02	1.31	1.35
17	W	11	A	C5-C4	-5.01	1.35	1.38
17	W	40	C	P-O5'	-5.01	1.54	1.59
1	a	565	G	C2-N3	5.01	1.36	1.32
11	2	2283	G	C8-N7	5.00	1.33	1.30

All (305) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	2845	A	N1-C6-N6	39.32	142.19	118.60
13	7	2845	A	C6-N1-C2	38.58	141.75	118.60
13	7	2845	A	C5-C6-N1	-33.94	100.73	117.70
13	7	2845	A	N1-C2-N3	-22.70	117.95	129.30
17	W	54	U	C5-C6-N1	13.53	129.47	122.70
13	7	2845	A	C5-C6-N6	-12.67	113.56	123.70
17	W	43	A	C8-N9-C4	-12.66	100.74	105.80
17	W	43	A	N1-C2-N3	-11.48	123.56	129.30
17	W	43	A	C2-N3-C4	10.85	116.02	110.60
17	W	37	A	C5-N7-C8	10.82	109.31	103.90
17	W	74	C	N3-C4-C5	-10.49	117.70	121.90
11	2	2195	C	N3-C4-C5	10.38	126.05	121.90
11	2	2289	U	C2-N3-C4	-10.07	120.96	127.00
17	W	37	A	N7-C8-N9	-10.04	108.78	113.80
17	W	31	G	C5-C6-O6	-9.92	122.65	128.60
11	2	2245	C	C6-N1-C2	-9.86	116.36	120.30
11	2	2283	G	C8-N9-C4	-9.85	102.46	106.40
17	W	18	G	C5-C6-N1	9.55	116.28	111.50
17	W	12	G	C2-N3-C4	9.52	116.66	111.90
11	2	2278	C	N1-C2-O2	9.47	124.58	118.90
17	W	72	A	C5-C6-N1	9.38	122.39	117.70
17	W	61	C	N3-C4-C5	-9.22	118.21	121.90
17	W	1	C	C6-N1-C2	-9.11	116.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	W	18	G	C5-C6-O6	-8.98	123.21	128.60
11	2	2277	C	C5-C6-N1	-8.95	116.53	121.00
17	W	66	C	C6-N1-C2	8.95	123.88	120.30
17	W	31	G	C2-N3-C4	8.91	116.35	111.90
13	7	2835	U	C2-N1-C1'	8.88	128.35	117.70
7	h	1714	U	N1-C1'-C2'	8.79	125.42	114.00
17	W	76	A	N1-C6-N6	8.73	123.84	118.60
11	2	2247	G	C5-C6-O6	-8.71	123.37	128.60
17	W	43	A	N9-C4-C5	8.66	109.27	105.80
11	2	2302	G	N1-C6-O6	-8.64	114.72	119.90
17	W	6	G	C4-C5-N7	8.61	114.25	110.80
13	7	2828	G	N1-C6-O6	8.47	124.98	119.90
13	7	2867	C	N1-C2-O2	-8.46	113.82	118.90
13	7	2828	G	C5-C6-O6	-8.40	123.56	128.60
11	2	2283	G	N3-C2-N2	-8.38	114.03	119.90
17	W	68	C	C6-N1-C2	-8.38	116.95	120.30
17	W	49	G	N7-C8-N9	8.37	117.29	113.10
17	W	18	G	C5-N7-C8	-8.33	100.13	104.30
17	W	51	C	C2-N3-C4	8.32	124.06	119.90
17	W	16	C	C6-N1-C2	8.31	123.63	120.30
11	2	2247	G	C4-C5-N7	8.28	114.11	110.80
13	7	2837	A	N1-C6-N6	-8.28	113.63	118.60
11	2	2303	A	C8-N9-C4	8.23	109.09	105.80
17	W	2	G	N9-C4-C5	-8.04	102.19	105.40
17	W	9	G	C5-N7-C8	7.92	108.26	104.30
17	W	59	A	C8-N9-C4	7.92	108.97	105.80
17	W	9	G	C4-C5-N7	-7.89	107.64	110.80
17	W	63	G	N3-C4-N9	7.85	130.71	126.00
17	W	15	G	N1-C6-O6	-7.84	115.20	119.90
17	W	70	G	C4-C5-N7	-7.82	107.67	110.80
17	W	6	G	C5-C6-O6	-7.78	123.93	128.60
11	2	2283	G	N1-C6-O6	7.76	124.56	119.90
11	2	2290	C	N1-C2-O2	-7.75	114.25	118.90
17	W	76	A	C5-C6-N1	-7.75	113.82	117.70
17	W	18	G	C4-C5-N7	7.74	113.90	110.80
17	W	21	A	C2-N3-C4	7.74	114.47	110.60
13	7	2851	A	N1-C6-N6	-7.70	113.98	118.60
17	W	54	U	C4-C5-C6	-7.68	115.09	119.70
13	7	2835	U	C5-C4-O4	-7.67	121.30	125.90
17	W	17	C	C5-C6-N1	7.65	124.82	121.00
17	W	52	G	C5-C6-N1	7.63	115.32	111.50
17	W	73	A	N7-C8-N9	-7.60	110.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	2247	G	C6-C5-N7	-7.59	125.84	130.40
11	2	2277	C	C2-N3-C4	-7.58	116.11	119.90
17	W	62	C	C6-N1-C2	7.57	123.33	120.30
13	7	2835	U	N3-C4-O4	7.55	124.68	119.40
17	W	62	C	C4-C5-C6	7.54	121.17	117.40
17	W	38	A	N9-C4-C5	-7.53	102.79	105.80
17	W	72	A	N1-C6-N6	-7.53	114.08	118.60
11	2	2283	G	N3-C4-N9	-7.50	121.50	126.00
11	2	2201	G	N1-C6-O6	7.47	124.38	119.90
17	W	4	G	O4'-C1'-N9	7.38	114.11	108.20
17	W	5	G	N9-C4-C5	-7.38	102.45	105.40
11	2	2241	U	C5-C4-O4	7.37	130.32	125.90
17	W	62	C	C5-C6-N1	-7.35	117.33	121.00
17	W	24	U	C5-C4-O4	7.30	130.28	125.90
17	W	17	C	C3'-C2'-C1'	7.27	107.32	101.50
11	2	2302	G	C6-C5-N7	7.24	134.75	130.40
17	W	8	U	C6-N1-C2	-7.24	116.66	121.00
17	W	5	G	C8-N9-C4	7.23	109.29	106.40
17	W	53	G	C6-N1-C2	7.23	129.44	125.10
17	W	49	G	C8-N9-C4	-7.20	103.52	106.40
17	W	55	U	C5-C6-N1	7.17	126.29	122.70
11	2	2267	C	N1-C2-O2	-7.12	114.63	118.90
11	2	2247	G	N1-C6-O6	7.03	124.12	119.90
17	W	6	G	N9-C4-C5	-7.00	102.60	105.40
17	W	31	G	N1-C2-N3	-6.93	119.74	123.90
17	W	12	G	C5-C6-N1	6.91	114.95	111.50
4	g	1172	G	N9-C1'-C2'	6.91	122.98	114.00
11	2	2248	C	N1-C2-O2	-6.87	114.78	118.90
11	2	2283	G	N7-C8-N9	6.83	116.52	113.10
11	2	2277	C	N1-C2-O2	-6.81	114.82	118.90
2	c	981	A	N9-C1'-C2'	6.80	122.84	114.00
17	W	31	G	N3-C4-N9	6.78	130.07	126.00
13	7	2824	G	C6-N1-C2	6.76	129.16	125.10
13	7	2830	G	C5-C6-N1	-6.74	108.13	111.50
1	a	588	A	N9-C1'-C2'	6.71	122.72	114.00
17	W	61	C	C4-C5-C6	6.70	120.75	117.40
11	2	2304	C	C6-N1-C2	-6.70	117.62	120.30
17	W	23	C	O4'-C1'-N1	6.62	113.50	108.20
17	W	75	C	C4-C5-C6	6.62	120.71	117.40
1	a	559	C	N1-C1'-C2'	6.60	122.58	114.00
11	2	2289	U	N3-C4-C5	6.54	118.52	114.60
11	2	2278	C	N1-C2-N3	-6.53	114.63	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	W	28	C	O4'-C1'-N1	6.53	113.43	108.20
17	W	22	G	O4'-C1'-N9	6.52	113.41	108.20
17	W	61	C	N3-C4-N4	6.51	122.56	118.00
11	2	2277	C	C6-N1-C2	6.50	122.90	120.30
17	W	55	U	N1-C2-N3	-6.45	111.03	114.90
13	7	2845	A	C2-N3-C4	-6.45	107.38	110.60
17	W	1	C	C5-C6-N1	6.43	124.22	121.00
17	W	66	C	C2-N3-C4	6.42	123.11	119.90
17	W	15	G	N3-C4-C5	-6.41	125.39	128.60
14	B	56	PRO	N-CA-CB	6.40	110.98	103.30
13	7	2847	A	C8-N9-C4	-6.40	103.24	105.80
1	a	565	G	N3-C2-N2	6.40	124.38	119.90
17	W	68	C	C5-C6-N1	6.37	124.19	121.00
13	7	2865	U	N1-C2-O2	-6.32	118.38	122.80
11	2	2218	G	C5-C6-N1	6.31	114.66	111.50
17	W	1	C	C5-C4-N4	6.31	124.62	120.20
17	W	37	A	C5-C6-N1	-6.30	114.55	117.70
17	W	52	G	C4-C5-C6	-6.30	115.02	118.80
17	W	15	G	C5-C6-O6	6.28	132.37	128.60
17	W	75	C	O5'-P-OP1	-6.28	100.04	105.70
11	2	2248	C	C6-N1-C2	6.27	122.81	120.30
13	7	2857	C	N3-C4-C5	6.25	124.40	121.90
4	g	1172	G	C2'-C3'-O3'	6.25	123.70	113.70
17	W	64	G	N3-C2-N2	-6.25	115.53	119.90
17	W	4	G	N9-C4-C5	6.21	107.88	105.40
17	W	26	G	C2-N3-C4	-6.20	108.80	111.90
11	2	2278	C	C6-N1-C1'	-6.20	113.37	120.80
17	W	71	C	N1-C2-N3	-6.18	114.87	119.20
11	2	2278	C	C2-N1-C1'	6.18	125.60	118.80
17	W	76	A	C4-C5-C6	6.14	120.07	117.00
17	W	65	C	N1-C2-O2	-6.14	115.22	118.90
13	7	2837	A	C8-N9-C4	6.12	108.25	105.80
1	a	574	A	N9-C1'-C2'	6.12	121.96	114.00
11	2	2280	A	C8-N9-C4	-6.12	103.35	105.80
13	7	2837	A	N7-C8-N9	-6.11	110.75	113.80
17	W	71	C	C2-N3-C4	6.11	122.95	119.90
17	W	13	C	C5-C4-N4	-6.08	115.94	120.20
17	W	72	A	C4-C5-C6	-6.07	113.97	117.00
17	W	69	C	N1-C1'-C2'	-6.06	105.33	112.00
14	B	61	PRO	N-CA-CB	6.05	110.56	103.30
17	W	76	A	C4-C5-N7	-6.05	107.68	110.70
11	2	2289	U	C5-C6-N1	-6.04	119.68	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	W	20	U	N1-C2-O2	6.04	127.03	122.80
14	B	135	PRO	N-CA-CB	6.04	110.54	103.30
11	2	2278	C	C2-N3-C4	6.03	122.91	119.90
13	7	2869	U	N3-C2-O2	-6.02	117.98	122.20
11	2	2196	C	C6-N1-C2	-6.01	117.89	120.30
14	B	121	PRO	N-CA-CB	6.01	110.51	103.30
11	2	2194	G	C8-N9-C4	6.01	108.80	106.40
11	2	2283	G	C5-N7-C8	-6.01	101.30	104.30
17	W	56	C	C5-C4-N4	-6.00	116.00	120.20
13	7	2835	U	C6-N1-C1'	-6.00	112.81	121.20
17	W	74	C	C3'-C2'-C1'	5.99	106.29	101.50
17	W	19	G	C8-N9-C4	5.97	108.79	106.40
17	W	10	G	C8-N9-C4	5.97	108.79	106.40
17	W	37	A	C8-N9-C4	5.97	108.19	105.80
17	W	12	G	C5-C6-O6	-5.96	125.02	128.60
17	W	18	G	O4'-C1'-N9	-5.95	103.44	108.20
14	B	126	PRO	N-CA-CB	5.94	110.43	103.30
17	W	57	A	C5-C6-N1	5.92	120.66	117.70
13	7	2868	U	N3-C2-O2	5.92	126.35	122.20
17	W	21	A	N3-C4-N9	5.92	132.14	127.40
17	W	8	U	C2-N3-C4	5.91	130.54	127.00
17	W	61	C	C2-N3-C4	5.90	122.85	119.90
17	W	63	G	C6-C5-N7	-5.90	126.86	130.40
11	2	2303	A	N9-C4-C5	-5.88	103.45	105.80
14	B	43	PRO	N-CA-CB	5.88	110.36	103.30
14	B	137	PRO	N-CA-CB	5.86	110.33	103.30
13	7	2867	C	N3-C2-O2	5.85	125.99	121.90
17	W	59	A	N1-C2-N3	-5.85	126.38	129.30
11	2	2201	G	C5-C6-O6	-5.84	125.09	128.60
14	B	212	PRO	N-CA-CB	5.84	110.31	103.30
17	W	22	G	N3-C4-C5	5.83	131.52	128.60
14	B	59	PRO	N-CA-CB	5.82	110.28	103.30
17	W	44	A	N9-C4-C5	-5.82	103.47	105.80
17	W	44	A	O4'-C1'-N9	-5.81	103.55	108.20
11	2	2241	U	C6-N1-C1'	5.80	129.32	121.20
11	2	2302	G	C5-C6-N1	5.80	114.40	111.50
17	W	66	C	N1-C2-N3	-5.79	115.14	119.20
17	W	71	C	C6-N1-C2	5.78	122.61	120.30
17	W	48	C	N1-C2-O2	-5.77	115.44	118.90
17	W	18	G	C2-N3-C4	5.76	114.78	111.90
17	W	51	C	C4'-C3'-C2'	5.76	108.36	102.60
17	W	70	G	C5-N7-C8	5.75	107.17	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	2283	G	N1-C2-N2	5.75	121.37	116.20
11	2	2290	C	C2-N3-C4	-5.75	117.03	119.90
17	W	10	G	N9-C4-C5	-5.74	103.10	105.40
11	2	2302	G	N3-C4-N9	-5.73	122.56	126.00
17	W	12	G	N9-C4-C5	-5.73	103.11	105.40
1	a	558	G	N9-C1'-C2'	5.73	121.45	114.00
17	W	55	U	O4'-C1'-N1	5.72	112.78	108.20
17	W	50	U	N3-C4-O4	-5.71	115.40	119.40
11	2	2283	G	C2-N3-C4	-5.71	109.05	111.90
17	W	64	G	N1-C2-N3	5.70	127.32	123.90
13	7	2837	A	C4-C5-N7	-5.70	107.85	110.70
17	W	50	U	C4-C5-C6	-5.70	116.28	119.70
11	2	2290	C	N3-C4-C5	5.68	124.17	121.90
17	W	58	A	N9-C4-C5	-5.68	103.53	105.80
11	2	2248	C	N3-C2-O2	5.67	125.87	121.90
17	W	18	G	C4-C5-C6	-5.67	115.40	118.80
1	a	552	C	N1-C1'-C2'	5.66	121.36	114.00
17	W	6	G	C5-N7-C8	-5.65	101.47	104.30
1	a	565	G	N1-C2-N2	-5.64	111.12	116.20
11	2	2301	U	C6-N1-C2	5.64	124.38	121.00
17	W	10	G	C4-C5-N7	5.64	113.05	110.80
17	W	73	A	C8-N9-C4	5.63	108.05	105.80
17	W	13	C	O4'-C1'-N1	-5.60	103.72	108.20
11	2	2196	C	N3-C4-C5	5.59	124.14	121.90
17	W	44	A	C4-C5-N7	5.59	113.50	110.70
17	W	8	U	N3-C4-C5	-5.59	111.25	114.60
11	2	2197	C	N3-C2-O2	5.58	125.81	121.90
11	2	2300	G	C8-N9-C1'	-5.56	119.77	127.00
11	2	2246	G	C5-C6-N1	5.56	114.28	111.50
13	7	2853	A	N1-C6-N6	5.56	121.93	118.60
17	W	63	G	N7-C8-N9	5.53	115.87	113.10
17	W	44	A	C2-N3-C4	-5.53	107.83	110.60
17	W	13	C	N3-C4-N4	5.53	121.87	118.00
11	2	2241	U	N1-C2-N3	5.52	118.21	114.90
11	2	2301	U	N3-C2-O2	5.52	126.06	122.20
17	W	64	G	C6-N1-C2	-5.51	121.79	125.10
17	W	75	C	N1-C2-O2	-5.51	115.59	118.90
17	W	17(A)	U	C2-N3-C4	5.50	130.30	127.00
17	W	64	G	C8-N9-C4	-5.49	104.20	106.40
17	W	6	G	C4-C5-C6	-5.49	115.51	118.80
17	W	23	C	N3-C4-C5	-5.49	119.71	121.90
17	W	21	A	C1'-O4'-C4'	-5.48	105.51	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	W	63	G	N3-C4-C5	-5.48	125.86	128.60
17	W	4	G	N9-C1'-C2'	-5.48	105.97	112.00
17	W	42	G	N1-C6-O6	-5.47	116.62	119.90
13	7	2830	G	C2-N3-C4	-5.47	109.17	111.90
17	W	50	U	N3-C4-C5	5.47	117.88	114.60
17	W	53	G	C5-C6-N1	-5.46	108.77	111.50
11	2	2274	U	N3-C2-O2	-5.45	118.38	122.20
11	2	2195	C	C5-C4-N4	-5.45	116.39	120.20
17	W	65	C	N3-C2-O2	5.43	125.70	121.90
17	W	31	G	C5-N7-C8	5.43	107.01	104.30
17	W	74	C	C4-C5-C6	5.43	120.11	117.40
11	2	2289	U	C5-C4-O4	-5.42	122.65	125.90
11	2	2301	U	N1-C2-O2	-5.41	119.01	122.80
17	W	17	C	C4-C5-C6	-5.41	114.70	117.40
17	W	18	G	C3'-C2'-C1'	5.41	105.83	101.50
17	W	12	G	N3-C4-N9	5.41	129.24	126.00
11	2	2283	G	N3-C4-C5	5.41	131.30	128.60
17	W	20	U	N3-C4-O4	-5.41	115.62	119.40
17	W	72	A	C6-C5-N7	5.40	136.08	132.30
11	2	2194	G	N7-C8-N9	-5.39	110.41	113.10
17	W	68	C	N1-C2-N3	5.38	122.96	119.20
13	7	2869	U	C2-N1-C1'	5.37	124.15	117.70
17	W	31	G	C5-C6-N1	5.37	114.18	111.50
17	W	74	C	N3-C4-N4	5.33	121.73	118.00
17	W	67	C	C6-N1-C2	-5.33	118.17	120.30
11	2	2275	A	C5-C6-N1	-5.31	115.05	117.70
11	2	2303	A	C5-C6-N1	5.31	120.36	117.70
11	2	2247	G	C5-N7-C8	-5.30	101.65	104.30
17	W	71	C	C4-C5-C6	-5.30	114.75	117.40
13	7	2859	U	N3-C2-O2	5.29	125.91	122.20
17	W	3	C	C5-C6-N1	-5.29	118.36	121.00
17	W	5	G	N7-C8-N9	-5.29	110.46	113.10
17	W	59	A	N1-C6-N6	-5.28	115.43	118.60
17	W	38	A	N7-C8-N9	5.28	116.44	113.80
17	W	43	A	N7-C8-N9	5.28	116.44	113.80
17	W	65	C	C4-C5-C6	5.28	120.04	117.40
17	W	15	G	C6-N1-C2	-5.28	121.94	125.10
17	W	70	G	C6-C5-N7	5.27	133.56	130.40
17	W	21	A	N3-C4-C5	-5.27	123.11	126.80
17	W	71	C	C5'-C4'-C3'	-5.27	107.57	116.00
11	2	2246	G	N3-C4-N9	5.25	129.15	126.00
17	W	37	A	C4-C5-C6	5.24	119.62	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	W	4	G	C3'-C2'-C1'	5.22	105.68	101.50
17	W	24	U	P-O5'-C5'	-5.21	112.56	120.90
17	W	44	A	C5-N7-C8	-5.21	101.29	103.90
17	W	21	A	N1-C6-N6	-5.20	115.48	118.60
17	W	4	G	C5'-C4'-C3'	-5.20	107.68	116.00
17	W	20	U	O4'-C1'-N1	5.20	112.36	108.20
17	W	24	U	N3-C2-O2	-5.18	118.57	122.20
17	W	14	A	C6-N1-C2	5.18	121.71	118.60
17	W	32	C	N1-C2-O2	-5.14	115.81	118.90
17	W	74	C	C2-N3-C4	5.14	122.47	119.90
17	W	31	G	N1-C6-O6	5.14	122.98	119.90
11	2	2215	A	C2-N3-C4	-5.14	108.03	110.60
17	W	17(A)	U	N1-C2-O2	5.13	126.39	122.80
17	W	71	C	C4'-C3'-C2'	-5.12	97.48	102.60
17	W	31	G	N3-C4-C5	-5.10	126.05	128.60
17	W	53	G	C4-C5-N7	5.08	112.83	110.80
11	2	2281	A	C4-C5-C6	5.07	119.53	117.00
17	W	56	C	N3-C4-C5	5.07	123.93	121.90
1	a	559	C	O4'-C1'-N1	5.06	112.25	108.20
13	7	2828	G	C8-N9-C1'	-5.05	120.44	127.00
8	S	131	THR	N-CA-C	5.04	124.61	111.00
13	7	2869	U	C6-N1-C2	-5.04	117.97	121.00
17	W	69	C	C2-N3-C4	5.04	122.42	119.90
17	W	59	A	N9-C4-C5	-5.04	103.78	105.80
17	W	2	G	N3-C4-N9	5.02	129.01	126.00
11	2	2261	G	N1-C6-O6	5.02	122.91	119.90
13	7	2824	G	C5-C6-N1	-5.01	109.00	111.50
17	W	10	G	C5-C6-O6	-5.01	125.60	128.60
17	W	11	A	N1-C6-N6	5.00	121.60	118.60
11	2	2290	C	C5-C6-N1	-5.00	118.50	121.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	W	15	G	Sidechain
17	W	29	G	Sidechain
17	W	33	U	Sidechain
17	W	4	G	Sidechain
17	W	8	U	Sidechain
1	a	547	C	Sidechain
1	a	559	C	Sidechain

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Mol	Chain	Res	Type	Group
1	a	574	A	Sidechain
3	d	1545	A	Sidechain
4	g	1157	U	Sidechain
4	g	1158	U	Sidechain
7	h	1610	G	Sidechain
7	h	1714	U	Sidechain

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	
8	S	123/125 (98%)	90 (73%)	25 (20%)	8 (6%)	1	16
9	L	139/141 (99%)	106 (76%)	18 (13%)	15 (11%)	0	8
10	X	66/68 (97%)	48 (73%)	12 (18%)	6 (9%)	1	11
14	B	211/213 (99%)	76 (36%)	67 (32%)	68 (32%)	0	0
All	All	539/547 (98%)	320 (59%)	122 (23%)	97 (18%)	0	3

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	S	15	GLY
9	L	45	ALA
9	L	62	GLN
9	L	87	PRO
9	L	88	MET
9	L	89	ASP
9	L	107	GLY
9	L	108	ARG

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Mol	Chain	Res	Type
9	L	117	PRO
10	X	8	LEU
10	X	64	ALA
14	B	24	LYS
14	B	36	VAL
14	B	39	LYS
14	B	42	ASP
14	B	43	PRO
14	B	55	LEU
14	B	56	PRO
14	B	58	CYS
14	B	59	PRO
14	B	60	ARG
14	B	61	PRO
14	B	109	ALA
14	B	115	VAL
14	B	120	VAL
14	B	122	ARG
14	B	124	LEU
14	B	126	PRO
14	B	127	GLN
14	B	128	LEU
14	B	129	SER
14	B	135	PRO
14	B	143	ASP
14	B	151	VAL
14	B	174	MET
14	B	201	VAL
14	B	207	LYS
14	B	208	SER
14	B	209	SER
14	B	210	MET
14	B	212	PRO
8	S	31	GLU
8	S	33	LEU
9	L	35	GLY
9	L	54	GLU
9	L	76	ARG
9	L	138	LYS
10	X	24	LYS
14	B	25	LYS
14	B	26	ARG

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Mol	Chain	Res	Type
14	B	41	TYR
14	B	44	GLN
14	B	47	LYS
14	B	67	ILE
14	B	77	ALA
14	B	96	ASN
14	B	117	ILE
14	B	123	LEU
14	B	169	VAL
14	B	193	LEU
14	B	194	LEU
14	B	196	LYS
14	B	197	ASN
14	B	204	LEU
14	B	206	VAL
8	S	130	PRO
9	L	91	CYS
9	L	109	GLN
10	X	60	PRO
14	B	22	GLU
14	B	49	PHE
14	B	57	ASN
14	B	101	LYS
14	B	102	LYS
14	B	152	ARG
14	B	202	GLY
10	X	25	ASP
14	B	27	ASN
14	B	107	TYR
14	B	132	GLY
14	B	155	ILE
14	B	165	LEU
14	B	189	PHE
14	B	213	ALA
8	S	123	GLU
10	X	26	LYS
14	B	5	THR
14	B	45	ARG
14	B	92	LYS
14	B	108	ASN
14	B	154	THR
8	S	85	TYR

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Mol	Chain	Res	Type
8	S	104	GLY
14	B	69	GLY
9	L	110	GLY
14	B	65	ILE
8	S	53	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	S	105/105 (100%)	101 (96%)	4 (4%)	33	57
9	L	113/113 (100%)	102 (90%)	11 (10%)	8	27
10	X	57/57 (100%)	55 (96%)	2 (4%)	36	59
All	All	275/275 (100%)	258 (94%)	17 (6%)	22	43

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	S	66	ARG
8	S	83	THR
8	S	85	TYR
8	S	124	PHE
9	L	9	ILE
9	L	19	ARG
9	L	33	LEU
9	L	55	LYS
9	L	69	LYS
9	L	81	LYS
9	L	82	ILE
9	L	89	ASP
9	L	92	LEU
9	L	106	LEU
9	L	132	LEU
10	X	34	ARG
10	X	62	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
8	S	29	ASN
8	S	84	HIS
8	S	133	HIS
9	L	78	ASN
9	L	98	ASN
10	X	42	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	47/48 (97%)	15 (31%)	0
11	2	111/112 (99%)	54 (48%)	9 (8%)
12	3	11/12 (91%)	6 (54%)	1 (9%)
13	7	49/50 (98%)	29 (59%)	5 (10%)
15	Y	74/75 (98%)	20 (27%)	1 (1%)
16	y	2/3 (66%)	0	0
17	W	76/77 (98%)	17 (22%)	0
18	w	1/2 (50%)	0	0
2	c	16/17 (94%)	4 (25%)	0
3	d	6/7 (85%)	2 (33%)	0
4	g	30/31 (96%)	8 (26%)	0
5	G	12/13 (92%)	2 (16%)	1 (8%)
6	f	20/21 (95%)	5 (25%)	0
7	h	110/111 (99%)	12 (10%)	0
All	All	565/579 (97%)	174 (30%)	17 (3%)

All (174) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	544	G
1	a	547	C
1	a	548	A
1	a	552	C
1	a	553	A
1	a	554	U
1	a	559	C
1	a	560	C
1	a	568	G
1	a	573	A
1	a	574	A

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Mol	Chain	Res	Type
1	a	575	U
1	a	576	U
1	a	577	C
1	a	588	A
2	c	975	G
2	c	976	A
2	c	978	C
2	c	982	U
3	d	1545	A
3	d	1546	G
4	g	1155	A
4	g	1158	U
4	g	1163	U
4	g	1165	A
4	g	1166	A
4	g	1168	A
4	g	1169	C
4	g	1172	G
5	G	1430	C
5	G	1431	A
6	f	1242	G
6	f	1245	G
6	f	1246	C
6	f	1247	A
6	f	1256	C
7	h	1608	C
7	h	1609	C
7	h	1624	G
7	h	1649	U
7	h	1651	G
7	h	1652	A
7	h	1661	G
7	h	1674	A
7	h	1710	G
7	h	1713	G
7	h	1714	U
7	h	1715	A
11	2	2195	C
11	2	2201	G
11	2	2205	U
11	2	2206	G
11	2	2207	A

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Mol	Chain	Res	Type
11	2	2208	A
11	2	2209	U
11	2	2210	G
11	2	2211	U
11	2	2215	A
11	2	2222	A
11	2	2223	A
11	2	2224	A
11	2	2227	C
11	2	2237	C
11	2	2244	A
11	2	2247	G
11	2	2248	C
11	2	2249	G
11	2	2250	G
11	2	2252	A
11	2	2254	U
11	2	2255	A
11	2	2256	A
11	2	2257	C
11	2	2259	A
11	2	2260	U
11	2	2261	G
11	2	2262	A
11	2	2263	C
11	2	2264	U
11	2	2266	U
11	2	2270	A
11	2	2272	G
11	2	2273	G
11	2	2275	A
11	2	2276	G
11	2	2277	C
11	2	2280	A
11	2	2281	A
11	2	2282	U
11	2	2283	G
11	2	2286	U
11	2	2288	G
11	2	2290	C
11	2	2291	A
11	2	2292	U

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Mol	Chain	Res	Type
11	2	2295	A
11	2	2296	A
11	2	2297	U
11	2	2298	U
11	2	2299	A
11	2	2300	G
11	2	2303	A
12	3	2479	C
12	3	2484	A
12	3	2485	A
12	3	2486	A
12	3	2487	U
12	3	2488	A
13	7	2825	C
13	7	2826	U
13	7	2828	G
13	7	2829	U
13	7	2830	G
13	7	2833	A
13	7	2834	G
13	7	2835	U
13	7	2836	C
13	7	2838	A
13	7	2839	G
13	7	2840	C
13	7	2842	U
13	7	2843	U
13	7	2844	C
13	7	2845	A
13	7	2846	U
13	7	2847	A
13	7	2849	C
13	7	2850	G
13	7	2851	A
13	7	2852	C
13	7	2859	U
13	7	2860	U
13	7	2867	C
13	7	2870	C
13	7	2871	G
13	7	2872	A
13	7	2873	U

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Mol	Chain	Res	Type
15	Y	2	C
15	Y	9	A
15	Y	16	U
15	Y	17	C
15	Y	18	G
15	Y	19	G
15	Y	21	A
15	Y	23	A
15	Y	34	G
15	Y	42	C
15	Y	43	C
15	Y	47	U
15	Y	48	C
15	Y	52	G
15	Y	53	G
15	Y	70	G
15	Y	71	G
15	Y	72	C
15	Y	73	A
15	Y	74	C
17	W	4	G
17	W	5	G
17	W	8	U
17	W	17	C
17	W	17(A)	U
17	W	18	G
17	W	19	G
17	W	20	U
17	W	21	A
17	W	36	U
17	W	47	U
17	W	48	C
17	W	63	G
17	W	71	C
17	W	74	C
17	W	75	C
17	W	76	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	G	1430	C

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Mol	Chain	Res	Type
11	2	2211	U
11	2	2251	G
11	2	2254	U
11	2	2255	A
11	2	2270	A
11	2	2280	A
11	2	2281	A
11	2	2290	C
11	2	2297	U
12	3	2487	U
13	7	2834	G
13	7	2850	G
13	7	2851	A
13	7	2859	U
13	7	2872	A
15	Y	15	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 [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](#)

There are no chain breaks in this entry.

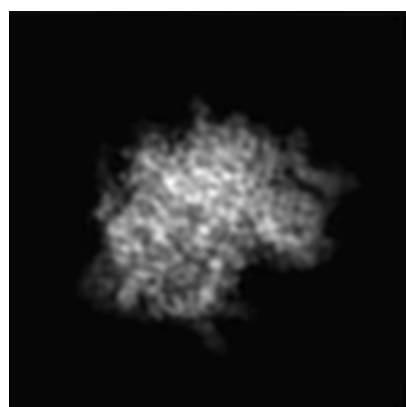
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5328. These allow visual inspection of the internal detail of the map and identification of artifacts.

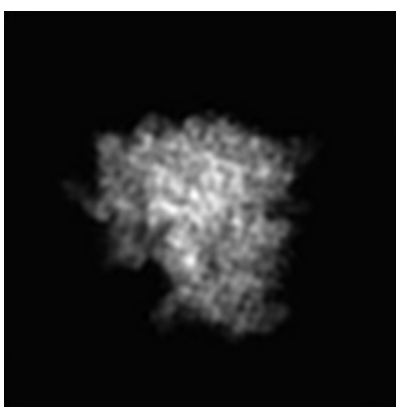
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

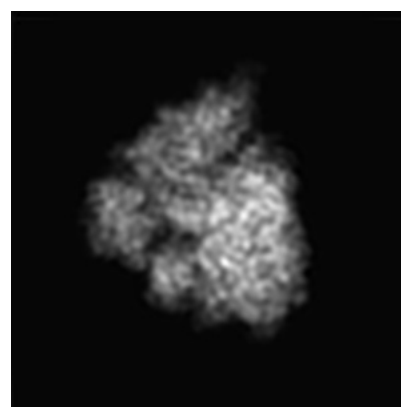
6.1.1 Primary map



X



Y

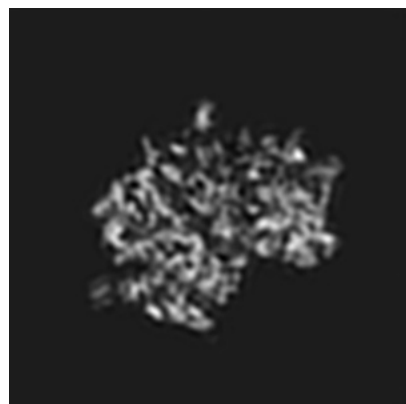


Z

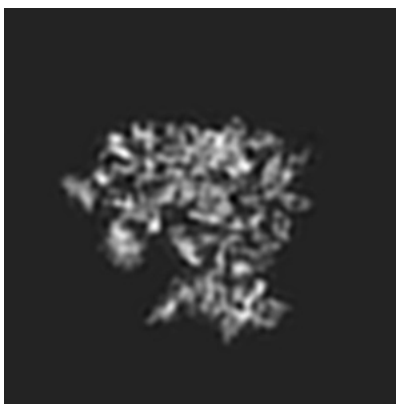
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

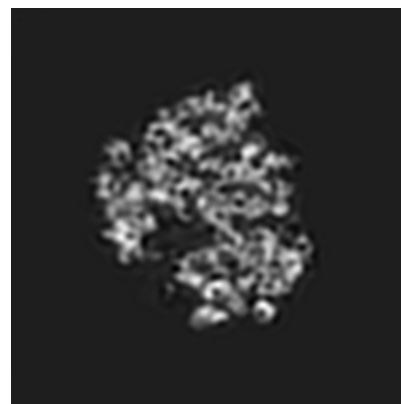
6.2.1 Primary map



X Index: 90



Y Index: 90

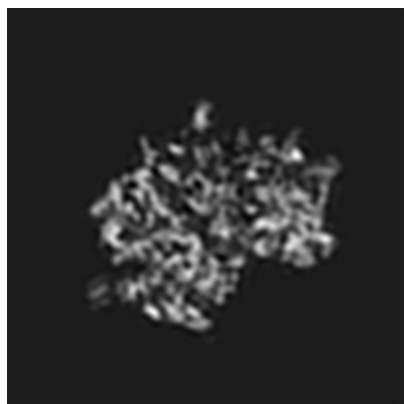


Z Index: 90

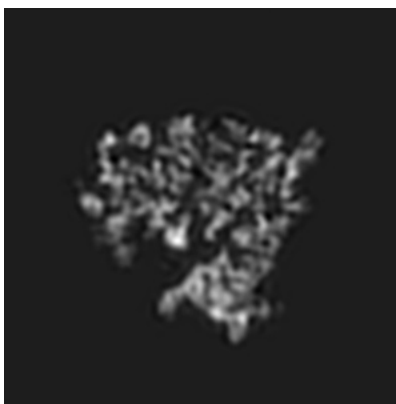
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 90



Y Index: 85



Z Index: 83

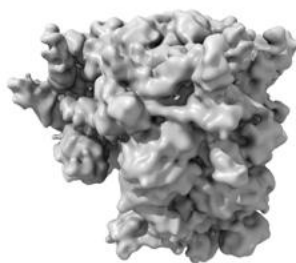
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

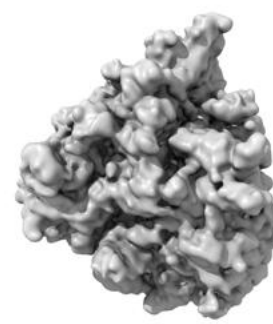
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1000.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

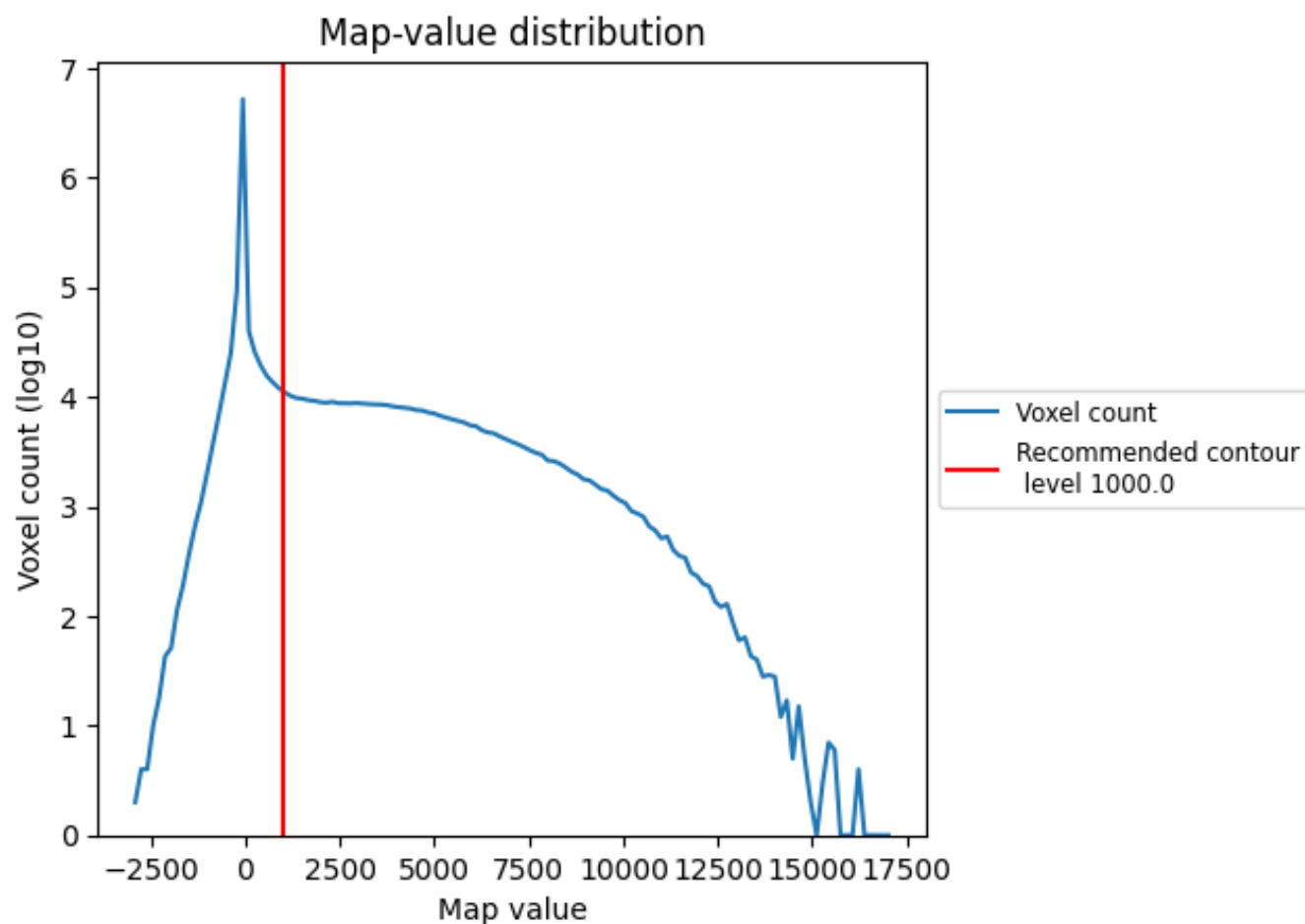
6.5 Mask visualisation

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

7 Map analysis [i](#)

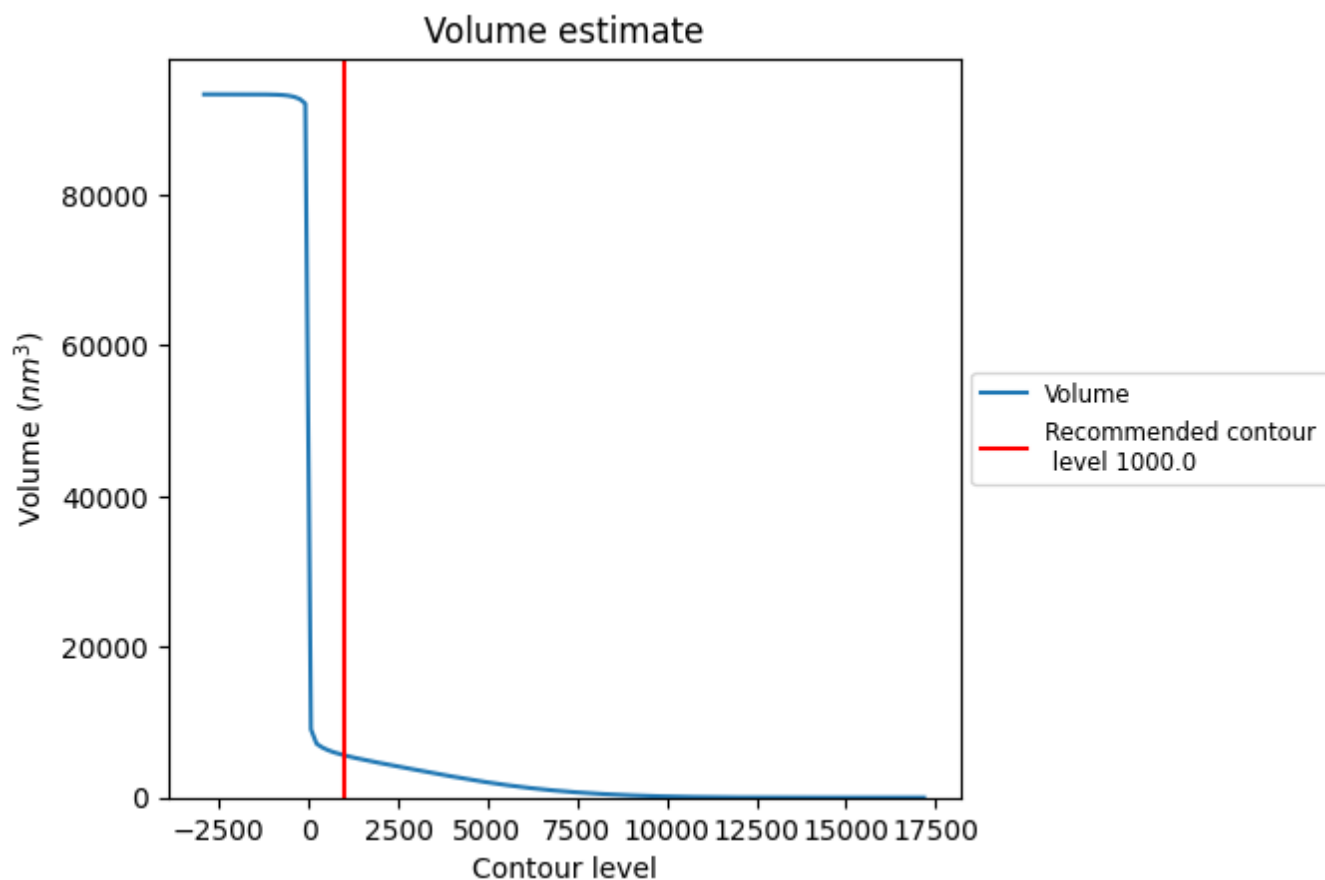
This section contains the results of statistical analysis of the map.

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.

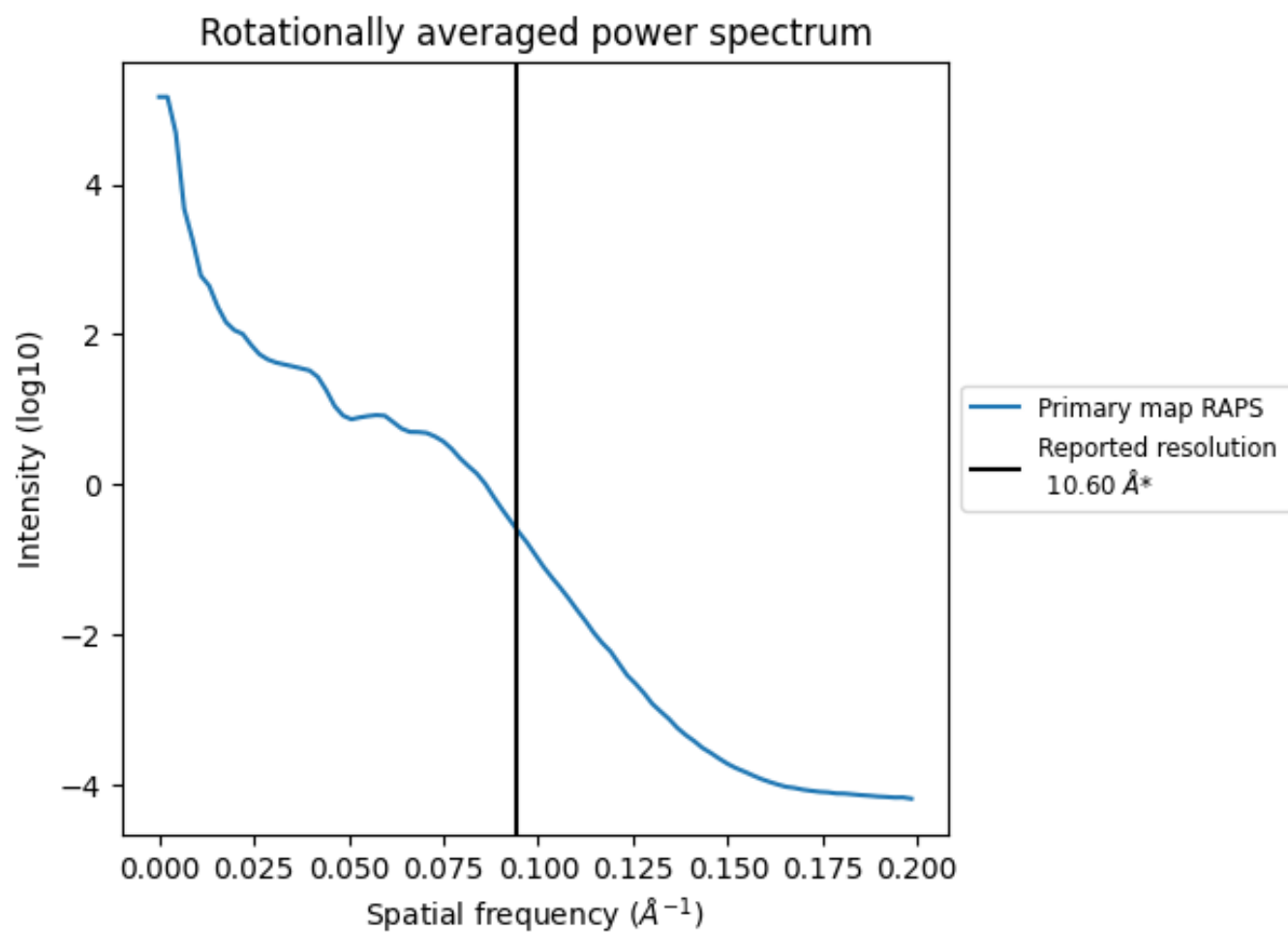
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5603 nm³; this corresponds to an approximate mass of 5061 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.094 Å⁻¹

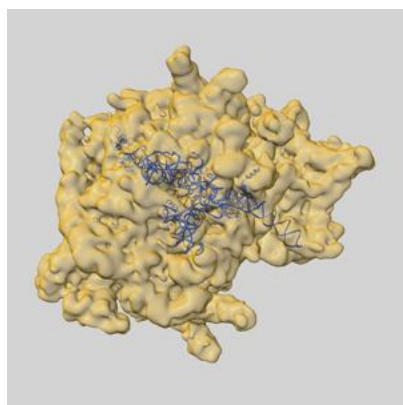
8 Fourier-Shell correlation

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

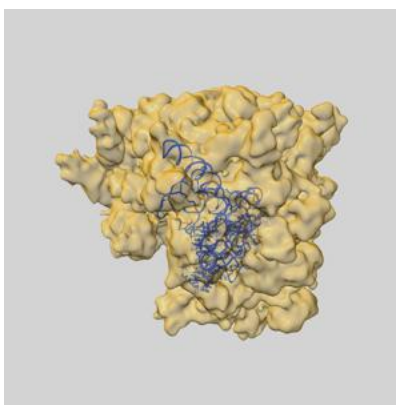
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5328 and PDB model 3J0P. Per-residue inclusion information can be found in section [3](#) on page [7](#).

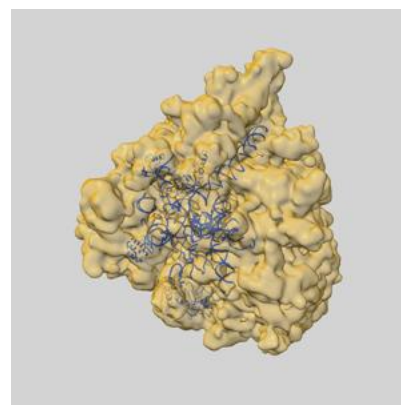
9.1 Map-model overlay [i](#)



X



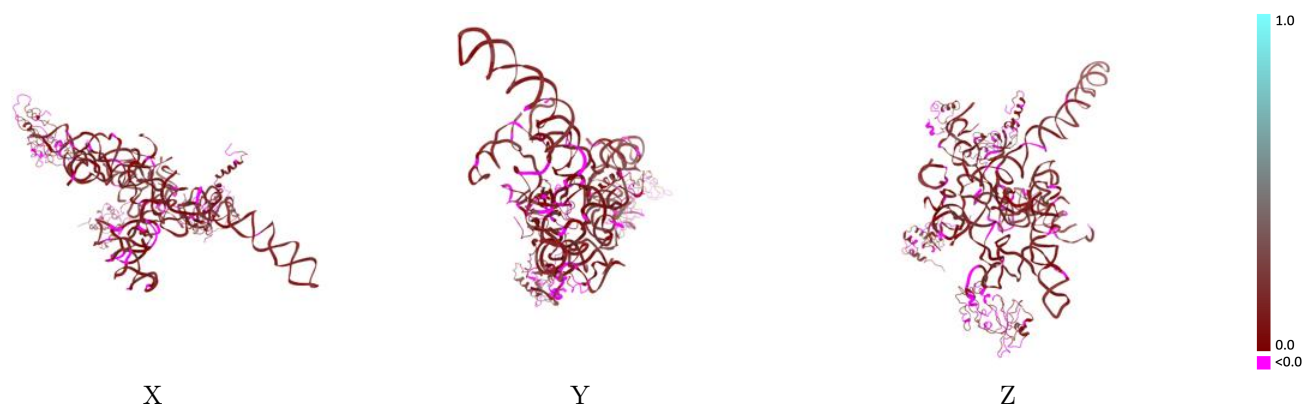
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1000.0 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](#)



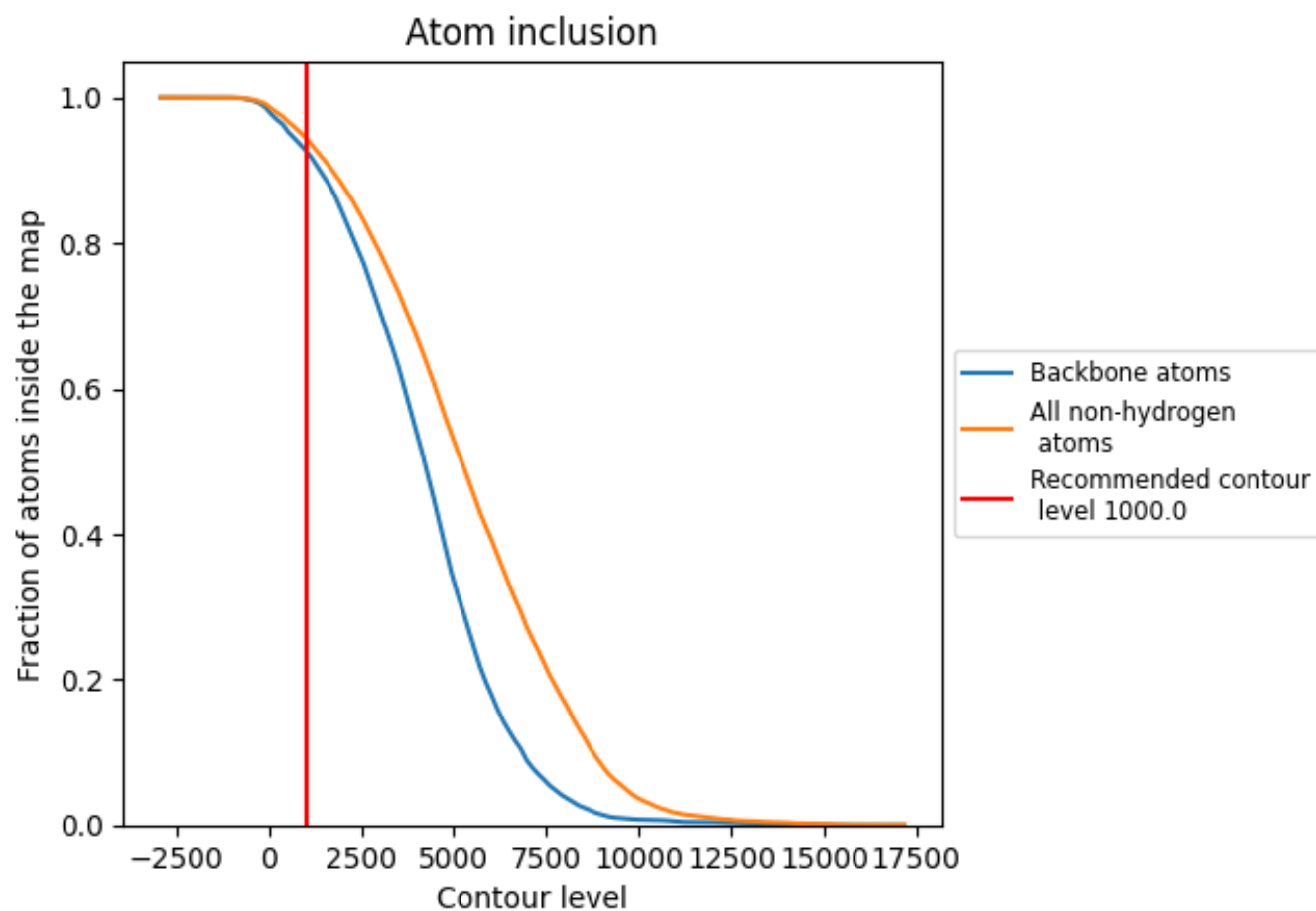
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1000.0).







































9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 95% 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 (1000.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9451	 0.0920
2	 0.9745	 0.1170
3	 0.8919	 0.0530
7	 0.9924	 0.1160
B	 0.8237	 0.0250
G	 1.0000	 0.1290
L	 0.9465	 0.0540
S	 0.9315	 0.0600
W	 0.9610	 0.1250
X	 0.7799	 0.0380
Y	 0.8929	 0.0770
a	 0.9922	 0.1050
c	 0.9779	 0.0990
d	 1.0000	 0.1180
f	 0.9978	 0.1130
g	 0.9985	 0.0880
h	 0.9679	 0.1070
w	 0.4773	 -0.1380
y	 1.0000	 0.1110

