



## Full wwPDB EM Validation Report ⓘ

Aug 20, 2022 – 08:56 am BST

PDB ID : 7ZHG  
EMDB ID : EMD-14731  
Title : High-resolution cryo-EM structure of *Pyrococcus abyssi* 30S ribosomal subunit bound to mRNA and initiator tRNA anticodon stem-loop  
Authors : Kazan, R.; Bourgeois, G.; Mechulam, Y.; Coureux, P.D.; Schmitt, E.  
Deposited on : 2022-04-06  
Resolution : 2.25 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

EMDB validation analysis : 0.0.1.dev8  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

# 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 2.25 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 64278 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 rRNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1497	Total	C	N	O	P	0	0
			32312	14418	5959	10438	1497		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	17	4AC	C	modified residue	GB 5457433
2	53	4AC	C	modified residue	GB 5457433
2	286	4AC	C	modified residue	GB 5457433
2	303	4AC	C	modified residue	GB 5457433
2	319	4AC	C	modified residue	GB 5457433
2	379	4AC	C	modified residue	GB 5457433
2	394	4AC	C	modified residue	GB 5457433
2	479	4AC	C	modified residue	GB 5457433
2	511	4AC	C	modified residue	GB 5457433
2	546	4AC	C	modified residue	GB 5457433
2	590	4AC	C	modified residue	GB 5457433
2	626	4AC	C	modified residue	GB 5457433
2	636	4AC	C	modified residue	GB 5457433
2	703	4AC	C	modified residue	GB 5457433
2	718	4AC	C	modified residue	GB 5457433
2	731	4AC	C	modified residue	GB 5457433
2	751	4AC	C	modified residue	GB 5457433
2	828	4AC	C	modified residue	GB 5457433
2	839	4AC	C	modified residue	GB 5457433
2	848	4AC	C	modified residue	GB 5457433
2	851	4AC	C	modified residue	GB 5457433
2	868	4AC	C	modified residue	GB 5457433
2	957	4AC	C	modified residue	GB 5457433
2	1028	4AC	C	modified residue	GB 5457433
2	1147	4AC	C	modified residue	GB 5457433
2	1184	4AC	C	modified residue	GB 5457433
2	1233	4AC	C	modified residue	GB 5457433
2	1239	4AC	C	modified residue	GB 5457433

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Chain	Residue	Modelled	Actual	Comment	Reference
2	1479	4AC	C	modified residue	GB 5457433

- Molecule 2 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	188	Total	C	N	O	S	0	0
			1531	993	268	266	4		

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	196	Total	C	N	O	S	0	0
			1571	1017	269	281	4		

- Molecule 4 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	57	Total	C	N	O	S	0	0
			449	285	80	76	8		

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	173	Total	C	N	O	S	0	0
			1452	913	280	255	4		

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	242	Total	C	N	O	S	0	0
			1983	1281	358	339	5		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	124	Total	C	N	O	S	0	0
			977	621	178	176	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	214	Total	C	N	O	S	0	0
			1725	1095	323	300	7		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	129	Total	C	N	O	S	0	0
			1034	668	184	180	2		

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	125	Total	C	N	O		0	0
			986	612	205	169			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	135	Total	C	N	O	S	0	0
			1073	673	207	189	4		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	100	Total	C	N	O	S	0	0
			809	502	157	147	3		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	127	Total	C	N	O	S	0	0
			955	591	190	172	2		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	146	Total	C	N	O	S	0	0
			1148	727	224	194	3		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	141	Total	C	N	O	S	0	0
			1134	712	224	193	5		

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	55	Total	C	N	O	S	0	0
			455	288	95	67	5		

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	151	Total	C	N	O	S	0	0
			1257	801	239	213	4		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	107	Total	C	N	O	S	0	0
			884	562	172	147	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	64	Total	C	N	O	S	0	0
			541	343	104	93	1		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	124	Total	C	N	O	S	0	0
			1007	641	191	168	7		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	149	Total	C	N	O	0	0
			1223	790	221	212		

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	V	96	Total	C	N	O	S	0
			808	528	129	148	3	0

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	W	61	Total	C	N	O	S	0
			470	294	91	80	5	0

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	65	Total	C	N	O		0
			516	316	103	97		0

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	49	Total	C	N	O	S	0
			400	257	76	62	5	0

- Molecule 27 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Z	196	Total	C	N	O	S	0
			1541	983	284	270	4	0

- Molecule 28 is a protein called 50S ribosomal protein L41e.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	0	36	Total	C	N	O	S	0
			343	218	84	39	2	0

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	122	Total	C	N	O	S	0	0
			933	594	156	180	3		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	17	Total	C	N	O	P	0	0
			368	164	67	120	17		

- Molecule 31 is a RNA chain called Met-tRNA<sup>i</sup>Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	19	Total	C	N	O	P	0	0
			406	182	74	131	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	0	A	-	engineered mutation	GB 1334604293
4	72	U	A	engineered mutation	GB 1334604293

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	2	85	Total	Mg	0
			85	85	
32	F	1	Total	Mg	0
			1	1	
32	K	1	Total	Mg	0
			1	1	
32	M	1	Total	Mg	0
			1	1	
32	5	1	Total	Mg	0
			1	1	
32	4	1	Total	Mg	0
			1	1	

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	C	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
33	F	1	Total 1	Zn 1	0
33	P	1	Total 1	Zn 1	0
33	R	1	Total 1	Zn 1	0
33	W	1	Total 1	Zn 1	0

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	2	1713	Total 1713	O 1713	0
34	A	1	Total 1	O 1	0
34	B	10	Total 10	O 10	0
34	C	1	Total 1	O 1	0
34	D	35	Total 35	O 35	0
34	E	23	Total 23	O 23	0
34	F	45	Total 45	O 45	0
34	H	20	Total 20	O 20	0
34	I	16	Total 16	O 16	0
34	J	16	Total 16	O 16	0
34	K	26	Total 26	O 26	0
34	L	13	Total 13	O 13	0
34	M	18	Total 18	O 18	0
34	N	33	Total 33	O 33	0
34	O	11	Total 11	O 11	0

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Mol	Chain	Residues	Atoms		AltConf
34	P	8	Total 8	O 8	0
34	Q	21	Total 21	O 21	0
34	R	7	Total 7	O 7	0
34	S	1	Total 1	O 1	0
34	T	5	Total 5	O 5	0
34	U	16	Total 16	O 16	0
34	V	2	Total 2	O 2	0
34	W	4	Total 4	O 4	0
34	X	1	Total 1	O 1	0
34	Z	2	Total 2	O 2	0
34	0	15	Total 15	O 15	0
34	5	8	Total 8	O 8	0
34	4	12	Total 12	O 12	0

MolProbity failed to run properly - this section is therefore empty.

### 3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1000000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	39	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.336	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0249	Depositor
Map size (Å)	371.52002, 371.52002, 371.52002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8600001, 0.8600001, 0.8600001	Depositor

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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

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### 4.3 Torsion angles [i](#)

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

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#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

69 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	5MC	2	1505	1,30	18,22,23	0.94	2 (11%)	26,32,35	1.16	3 (11%)
1	4AC	2	839	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	A2M	2	373	1	18,25,26	0.98	1 (5%)	18,36,39	1.35	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	2	774	1	19,22,23	1.22	2 (10%)	26,31,34	1.73	4 (15%)
1	5MC	2	1025	1	18,22,23	0.94	2 (11%)	26,32,35	1.15	3 (11%)
1	OMU	2	1177	1	19,22,23	1.23	2 (10%)	26,31,34	1.67	4 (15%)
1	MA6	2	1487	1	19,26,27	0.90	1 (5%)	18,38,41	1.41	3 (16%)
1	4AC	2	828	1	21,24,25	1.06	2 (9%)	29,34,37	1.30	4 (13%)
1	5MC	2	693	1	18,22,23	0.94	2 (11%)	26,32,35	1.10	3 (11%)
1	OMC	2	846	1	19,22,23	0.76	0	26,31,34	0.88	1 (3%)
1	OMU	2	830	1	19,22,23	1.27	4 (21%)	26,31,34	1.83	4 (15%)
1	4AC	2	848	1	21,24,25	1.06	2 (9%)	29,34,37	1.42	4 (13%)
1	4AC	2	53	1	21,24,25	1.08	2 (9%)	29,34,37	1.25	4 (13%)
1	OMU	2	787	1	19,22,23	1.20	2 (10%)	26,31,34	1.90	5 (19%)
1	4AC	2	1147	1	21,24,25	1.03	2 (9%)	29,34,37	1.33	4 (13%)
1	5MC	2	1202	1	18,22,23	0.95	2 (11%)	26,32,35	1.08	3 (11%)
1	OMG	2	873	1	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)
31	OMC	4	32	31	19,22,23	0.84	0	26,31,34	0.99	2 (7%)
1	4AC	2	319	1	21,24,25	1.07	2 (9%)	29,34,37	1.33	4 (13%)
1	MA6	2	1488	1	19,26,27	0.89	1 (5%)	18,38,41	1.34	2 (11%)
1	4AC	2	394	1	21,24,25	1.09	2 (9%)	29,34,37	1.27	4 (13%)
1	LHH	2	250	1	22,25,26	2.50	8 (36%)	29,35,38	1.24	4 (13%)
1	OMU	2	64	1	19,22,23	1.18	3 (15%)	26,31,34	1.74	4 (15%)
1	5MC	2	535	1	18,22,23	0.90	2 (11%)	26,32,35	1.20	4 (15%)
1	OMG	2	913	1	18,26,27	0.88	1 (5%)	19,38,41	1.20	2 (10%)
1	OMU	2	20	1	19,22,23	1.22	3 (15%)	26,31,34	1.74	5 (19%)
1	5MC	2	875	1	18,22,23	0.92	2 (11%)	26,32,35	1.12	3 (11%)
1	4AC	2	626	1	21,24,25	1.04	2 (9%)	29,34,37	1.30	4 (13%)
1	5MC	2	1496	1	18,22,23	0.94	2 (11%)	26,32,35	1.17	3 (11%)
1	4AC	2	1233	1	21,24,25	1.07	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	2	1184	1	21,24,25	0.99	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	2	286	1	21,24,25	1.06	2 (9%)	29,34,37	1.33	4 (13%)
1	OMG	2	1069	1	18,26,27	0.88	1 (5%)	19,38,41	1.09	2 (10%)
1	4AC	2	1028	1	21,24,25	1.05	2 (9%)	29,34,37	1.30	4 (13%)
1	OMC	2	1376	1	19,22,23	0.78	0	26,31,34	0.82	0
1	4AC	2	851	1	21,24,25	1.13	2 (9%)	29,34,37	1.25	3 (10%)
1	OMU	2	1380	1	19,22,23	1.21	2 (10%)	26,31,34	1.75	5 (19%)
1	OMG	2	467	1	18,26,27	0.92	1 (5%)	19,38,41	1.11	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4AC	2	511	1	21,24,25	1.09	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	2	636	1	21,24,25	1.07	2 (9%)	29,34,37	1.65	4 (13%)
1	4AC	2	957	1	21,24,25	1.06	2 (9%)	29,34,37	1.28	4 (13%)
1	4AC	2	868	1	21,24,25	1.10	2 (9%)	29,34,37	1.26	3 (10%)
1	B8H	2	938	1	19,22,23	0.76	0	22,32,35	1.40	3 (13%)
1	UR3	2	1467	1	19,22,23	0.95	1 (5%)	26,32,35	1.39	2 (7%)
1	OMG	2	471	1	18,26,27	0.92	1 (5%)	19,38,41	1.06	2 (10%)
1	OMG	2	934	1	18,26,27	0.95	1 (5%)	19,38,41	1.18	2 (10%)
1	4AC	2	731	1	21,24,25	1.06	2 (9%)	29,34,37	1.18	3 (10%)
1	OMC	2	1040	1	19,22,23	0.77	0	26,31,34	0.78	0
1	LHH	2	1041	1	22,25,26	2.50	8 (36%)	29,35,38	1.24	4 (13%)
1	4AC	2	703	1	21,24,25	1.09	3 (14%)	29,34,37	1.58	4 (13%)
1	5MC	2	1374	1	18,22,23	0.95	2 (11%)	26,32,35	1.11	3 (11%)
1	OMC	2	1036	1	19,22,23	0.79	0	26,31,34	0.87	1 (3%)
1	5MC	2	1498	1	18,22,23	0.94	2 (11%)	26,32,35	1.34	5 (19%)
1	4AC	2	17	1	21,24,25	1.07	2 (9%)	29,34,37	1.23	4 (13%)
1	4AC	2	1239	1	21,24,25	1.05	2 (9%)	29,34,37	1.30	4 (13%)
1	OMG	2	680	1	18,26,27	0.94	1 (5%)	19,38,41	1.05	2 (10%)
1	4AC	2	1479	1	21,24,25	1.11	2 (9%)	29,34,37	1.23	3 (10%)
1	4AC	2	718	1	21,24,25	1.06	2 (9%)	29,34,37	1.22	5 (17%)
1	4AC	2	379	1	21,24,25	1.06	2 (9%)	29,34,37	1.25	3 (10%)
1	4AC	2	751	1	21,24,25	1.05	2 (9%)	29,34,37	1.19	4 (13%)
1	4AC	2	479	1	21,24,25	1.05	2 (9%)	29,34,37	1.36	4 (13%)
1	OMG	2	519	1	18,26,27	0.90	1 (5%)	19,38,41	1.14	2 (10%)
1	4AC	2	303	1	21,24,25	1.10	2 (9%)	29,34,37	1.26	3 (10%)
1	OMC	2	129	1	19,22,23	0.77	0	26,31,34	0.79	0
1	6MZ	2	1469	32,1	18,25,26	0.83	1 (5%)	16,36,39	2.33	3 (18%)
1	4AC	2	546	1	21,24,25	1.05	2 (9%)	29,34,37	1.23	3 (10%)
1	4AC	2	590	1	21,24,25	1.07	2 (9%)	29,34,37	1.30	4 (13%)
1	OMG	2	657	1	18,26,27	0.93	1 (5%)	19,38,41	1.04	2 (10%)
1	OMC	2	773	1	19,22,23	0.82	0	26,31,34	0.97	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2	1505	1,30	-	0/7/25/26	0/2/2/2
1	4AC	2	839	1	-	0/11/29/30	0/2/2/2
1	A2M	2	373	1	-	0/5/27/28	0/3/3/3
1	OMU	2	774	1	-	0/9/27/28	0/2/2/2
1	5MC	2	1025	1	-	0/7/25/26	0/2/2/2
1	OMU	2	1177	1	-	0/9/27/28	0/2/2/2
1	MA6	2	1487	1	-	0/7/29/30	0/3/3/3
1	4AC	2	828	1	-	0/11/29/30	0/2/2/2
1	5MC	2	693	1	-	0/7/25/26	0/2/2/2
1	OMC	2	846	1	-	0/9/27/28	0/2/2/2
1	OMU	2	830	1	-	0/9/27/28	0/2/2/2
1	4AC	2	848	1	-	0/11/29/30	0/2/2/2
1	4AC	2	53	1	-	0/11/29/30	0/2/2/2
1	OMU	2	787	1	-	4/9/27/28	0/2/2/2
1	4AC	2	1147	1	-	0/11/29/30	0/2/2/2
1	5MC	2	1202	1	-	2/7/25/26	0/2/2/2
1	OMG	2	873	1	-	0/5/27/28	0/3/3/3
31	OMC	4	32	31	-	2/9/27/28	0/2/2/2
1	4AC	2	319	1	-	0/11/29/30	0/2/2/2
1	MA6	2	1488	1	-	1/7/29/30	0/3/3/3
1	4AC	2	394	1	-	0/11/29/30	0/2/2/2
1	LHH	2	250	1	-	0/13/31/32	0/2/2/2
1	OMU	2	64	1	-	0/9/27/28	0/2/2/2
1	5MC	2	535	1	-	0/7/25/26	0/2/2/2
1	OMG	2	913	1	-	0/5/27/28	0/3/3/3
1	OMU	2	20	1	-	4/9/27/28	0/2/2/2
1	5MC	2	875	1	-	0/7/25/26	0/2/2/2
1	4AC	2	626	1	-	0/11/29/30	0/2/2/2
1	5MC	2	1496	1	-	0/7/25/26	0/2/2/2
1	4AC	2	1233	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1184	1	-	0/11/29/30	0/2/2/2
1	4AC	2	286	1	-	0/11/29/30	0/2/2/2
1	OMG	2	1069	1	-	0/5/27/28	0/3/3/3
1	4AC	2	1028	1	-	0/11/29/30	0/2/2/2
1	OMC	2	1376	1	-	0/9/27/28	0/2/2/2
1	4AC	2	851	1	-	0/11/29/30	0/2/2/2
1	OMU	2	1380	1	-	0/9/27/28	0/2/2/2
1	OMG	2	467	1	-	0/5/27/28	0/3/3/3
1	4AC	2	511	1	-	0/11/29/30	0/2/2/2
1	4AC	2	636	1	-	0/11/29/30	0/2/2/2
1	4AC	2	957	1	-	0/11/29/30	0/2/2/2
1	4AC	2	868	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	B8H	2	938	1	-	0/7/25/26	0/2/2/2
1	UR3	2	1467	1	-	0/7/25/26	0/2/2/2
1	OMG	2	471	1	-	0/5/27/28	0/3/3/3
1	OMG	2	934	1	-	0/5/27/28	0/3/3/3
1	4AC	2	731	1	-	0/11/29/30	0/2/2/2
1	OMC	2	1040	1	-	0/9/27/28	0/2/2/2
1	LHH	2	1041	1	-	0/13/31/32	0/2/2/2
1	4AC	2	703	1	-	0/11/29/30	0/2/2/2
1	5MC	2	1374	1	-	0/7/25/26	0/2/2/2
1	OMC	2	1036	1	-	0/9/27/28	0/2/2/2
1	5MC	2	1498	1	-	4/7/25/26	0/2/2/2
1	4AC	2	17	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1239	1	-	0/11/29/30	0/2/2/2
1	OMG	2	680	1	-	0/5/27/28	0/3/3/3
1	4AC	2	1479	1	-	0/11/29/30	0/2/2/2
1	4AC	2	718	1	-	0/11/29/30	0/2/2/2
1	4AC	2	379	1	-	0/11/29/30	0/2/2/2
1	4AC	2	751	1	-	0/11/29/30	0/2/2/2
1	4AC	2	479	1	-	0/11/29/30	0/2/2/2
1	OMG	2	519	1	-	0/5/27/28	0/3/3/3
1	4AC	2	303	1	-	0/11/29/30	0/2/2/2
1	OMC	2	129	1	-	0/9/27/28	0/2/2/2
1	6MZ	2	1469	32,1	-	0/5/27/28	0/3/3/3
1	4AC	2	546	1	-	0/11/29/30	0/2/2/2
1	4AC	2	590	1	-	0/11/29/30	0/2/2/2
1	OMG	2	657	1	-	0/5/27/28	0/3/3/3
1	OMC	2	773	1	-	0/9/27/28	0/2/2/2

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	250	LHH	C4-N4	6.92	1.49	1.39
1	2	1041	LHH	C4-N4	6.81	1.49	1.39
1	2	1041	LHH	C7-N4	6.38	1.49	1.37
1	2	250	LHH	C7-N4	6.27	1.48	1.37
1	2	1041	LHH	O2-C2	-4.28	1.15	1.23
1	2	250	LHH	O2-C2	-4.21	1.15	1.23
1	2	303	4AC	C5-C4	3.29	1.47	1.40
1	2	868	4AC	C5-C4	3.26	1.47	1.40
1	2	851	4AC	C5-C4	3.26	1.47	1.40
1	2	1479	4AC	C5-C4	3.23	1.47	1.40
1	2	511	4AC	C5-C4	3.23	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	590	4AC	C5-C4	3.21	1.47	1.40
1	2	17	4AC	C5-C4	3.20	1.47	1.40
1	2	379	4AC	C5-C4	3.17	1.47	1.40
1	2	53	4AC	C5-C4	3.15	1.47	1.40
1	2	751	4AC	C5-C4	3.15	1.47	1.40
1	2	718	4AC	C5-C4	3.15	1.47	1.40
1	2	731	4AC	C5-C4	3.14	1.47	1.40
1	2	546	4AC	C5-C4	3.14	1.47	1.40
1	2	828	4AC	C5-C4	3.13	1.47	1.40
1	2	319	4AC	C5-C4	3.12	1.47	1.40
1	2	957	4AC	C5-C4	3.11	1.47	1.40
1	2	1028	4AC	C5-C4	3.10	1.47	1.40
1	2	286	4AC	C5-C4	3.10	1.47	1.40
1	2	1239	4AC	C5-C4	3.08	1.47	1.40
1	2	1233	4AC	C5-C4	3.03	1.47	1.40
1	2	703	4AC	C5-C4	3.01	1.47	1.40
1	2	626	4AC	C5-C4	3.01	1.47	1.40
1	2	479	4AC	C5-C4	3.01	1.47	1.40
1	2	394	4AC	C5-C4	3.00	1.47	1.40
1	2	848	4AC	C5-C4	3.00	1.47	1.40
1	2	839	4AC	C5-C4	2.99	1.47	1.40
1	2	1147	4AC	C5-C4	2.99	1.47	1.40
1	2	1202	5MC	C6-C5	2.89	1.39	1.34
1	2	636	4AC	C5-C4	2.86	1.47	1.40
1	2	1374	5MC	C6-C5	2.86	1.39	1.34
1	2	1177	OMU	C4-N3	-2.86	1.33	1.38
1	2	1496	5MC	C6-C5	2.84	1.39	1.34
1	2	830	OMU	C4-N3	-2.83	1.33	1.38
1	2	1184	4AC	C5-C4	2.82	1.46	1.40
1	2	1025	5MC	C6-C5	2.73	1.39	1.34
1	2	1498	5MC	C6-C5	2.73	1.39	1.34
1	2	1505	5MC	C6-C5	2.71	1.39	1.34
1	2	657	OMG	C6-N1	-2.70	1.33	1.37
1	2	787	OMU	C4-N3	-2.70	1.33	1.38
1	2	250	LHH	C6-C5	2.69	1.41	1.35
1	2	873	OMG	C6-N1	-2.67	1.33	1.37
1	2	851	4AC	C4-N3	-2.67	1.28	1.32
1	2	1380	OMU	C4-N3	-2.67	1.33	1.38
1	2	693	5MC	C6-C5	2.67	1.39	1.34
1	2	875	5MC	C6-C5	2.67	1.39	1.34
1	2	774	OMU	C4-N3	-2.65	1.33	1.38
1	2	680	OMG	C6-N1	-2.64	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1041	LHH	C6-C5	2.61	1.41	1.35
1	2	519	OMG	C6-N1	-2.59	1.34	1.37
1	2	467	OMG	C6-N1	-2.58	1.34	1.37
1	2	1177	OMU	C2-N3	-2.54	1.33	1.38
1	2	394	4AC	C4-N3	-2.53	1.28	1.32
1	2	535	5MC	C6-C5	2.53	1.38	1.34
1	2	20	OMU	C4-N3	-2.52	1.34	1.38
1	2	957	4AC	C4-N3	-2.51	1.28	1.32
1	2	934	OMG	C6-N1	-2.50	1.34	1.37
1	2	1469	6MZ	C5-C4	2.50	1.47	1.40
1	2	1069	OMG	C6-N1	-2.48	1.34	1.37
1	2	53	4AC	C4-N3	-2.44	1.28	1.32
1	2	511	4AC	C4-N3	-2.43	1.28	1.32
1	2	17	4AC	C4-N3	-2.41	1.28	1.32
1	2	471	OMG	C6-N1	-2.40	1.34	1.37
1	2	1041	LHH	C2-N1	-2.40	1.34	1.40
1	2	1487	MA6	C5-C4	2.39	1.47	1.40
1	2	379	4AC	C4-N3	-2.39	1.28	1.32
1	2	1025	5MC	C6-N1	-2.39	1.34	1.38
1	2	1488	MA6	C5-C4	2.39	1.47	1.40
1	2	718	4AC	C4-N3	-2.39	1.28	1.32
1	2	250	LHH	C2-N1	-2.38	1.34	1.40
1	2	64	OMU	C4-N3	-2.38	1.34	1.38
1	2	303	4AC	C4-N3	-2.37	1.28	1.32
1	2	830	OMU	C2-N3	-2.37	1.33	1.38
1	2	1479	4AC	C4-N3	-2.35	1.28	1.32
1	2	546	4AC	C4-N3	-2.35	1.28	1.32
1	2	373	A2M	C5-C4	2.34	1.47	1.40
1	2	286	4AC	C4-N3	-2.34	1.28	1.32
1	2	590	4AC	C4-N3	-2.33	1.28	1.32
1	2	828	4AC	C4-N3	-2.32	1.28	1.32
1	2	848	4AC	C4-N3	-2.31	1.28	1.32
1	2	787	OMU	C2-N3	-2.31	1.33	1.38
1	2	868	4AC	C4-N3	-2.30	1.28	1.32
1	2	731	4AC	C4-N3	-2.29	1.28	1.32
1	2	1239	4AC	C4-N3	-2.28	1.28	1.32
1	2	875	5MC	C6-N1	-2.27	1.34	1.38
1	2	913	OMG	C6-N1	-2.27	1.34	1.37
1	2	535	5MC	C6-N1	-2.26	1.34	1.38
1	2	20	OMU	C2-N3	-2.26	1.33	1.38
1	2	1380	OMU	C2-N3	-2.26	1.33	1.38
1	2	250	LHH	C6-N1	-2.25	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	693	5MC	C6-N1	-2.25	1.34	1.38
1	2	319	4AC	C4-N3	-2.24	1.28	1.32
1	2	703	4AC	C4-N3	-2.23	1.28	1.32
1	2	479	4AC	C4-N3	-2.23	1.28	1.32
1	2	1498	5MC	C6-N1	-2.21	1.34	1.38
1	2	1233	4AC	C4-N3	-2.21	1.29	1.32
1	2	1496	5MC	C6-N1	-2.20	1.34	1.38
1	2	64	OMU	C2-N3	-2.20	1.34	1.38
1	2	1028	4AC	C4-N3	-2.19	1.29	1.32
1	2	636	4AC	C4-N3	-2.19	1.29	1.32
1	2	751	4AC	C4-N3	-2.19	1.29	1.32
1	2	626	4AC	C4-N3	-2.17	1.29	1.32
1	2	1467	UR3	C2-N1	2.17	1.41	1.38
1	2	774	OMU	C2-N3	-2.17	1.34	1.38
1	2	830	OMU	C5-C4	-2.15	1.38	1.43
1	2	1374	5MC	C6-N1	-2.15	1.34	1.38
1	2	703	4AC	C4-N4	-2.14	1.36	1.39
1	2	1041	LHH	C2-N3	-2.14	1.32	1.36
1	2	1202	5MC	C6-N1	-2.13	1.34	1.38
1	2	1184	4AC	C4-N3	-2.13	1.29	1.32
1	2	1147	4AC	C4-N3	-2.11	1.29	1.32
1	2	250	LHH	CM7-C7	2.09	1.54	1.50
1	2	1505	5MC	C6-N1	-2.08	1.34	1.38
1	2	64	OMU	C5-C4	-2.08	1.39	1.43
1	2	830	OMU	C2-N1	2.08	1.41	1.38
1	2	1041	LHH	C6-N1	-2.07	1.33	1.38
1	2	20	OMU	C2-N1	2.06	1.41	1.38
1	2	250	LHH	C2-N3	-2.04	1.32	1.36
1	2	839	4AC	C4-N3	-2.03	1.29	1.32
1	2	1041	LHH	CM7-C7	2.02	1.54	1.50

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1469	6MZ	C2-N1-C6	7.21	122.78	116.59
1	2	703	4AC	O7-C7-N4	5.37	130.50	121.82
1	2	1467	UR3	C4-N3-C2	-5.36	119.51	124.56
1	2	636	4AC	O7-C7-N4	5.31	130.41	121.82
1	2	787	OMU	N3-C2-N1	5.01	121.54	114.89
1	2	787	OMU	C4-N3-C2	-4.97	120.03	126.58
1	2	938	B8H	C4-N3-C2	-4.83	121.10	127.35
1	2	830	OMU	N3-C2-N1	4.72	121.15	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	830	OMU	C4-N3-C2	-4.70	120.37	126.58
1	2	1380	OMU	C4-N3-C2	-4.68	120.40	126.58
1	2	20	OMU	C4-N3-C2	-4.60	120.52	126.58
1	2	64	OMU	C4-N3-C2	-4.58	120.54	126.58
1	2	303	4AC	O7-C7-N4	4.54	129.16	121.82
1	2	1380	OMU	N3-C2-N1	4.53	120.91	114.89
1	2	1233	4AC	O7-C7-N4	4.53	129.15	121.82
1	2	479	4AC	O7-C7-N4	4.51	129.12	121.82
1	2	774	OMU	C4-N3-C2	-4.48	120.67	126.58
1	2	1028	4AC	O7-C7-N4	4.48	129.06	121.82
1	2	1184	4AC	O7-C7-N4	4.44	129.00	121.82
1	2	1177	OMU	C4-N3-C2	-4.42	120.75	126.58
1	2	590	4AC	O7-C7-N4	4.41	128.96	121.82
1	2	848	4AC	O7-C7-N4	4.41	128.95	121.82
1	2	1239	4AC	O7-C7-N4	4.40	128.94	121.82
1	2	957	4AC	O7-C7-N4	4.39	128.93	121.82
1	2	286	4AC	O7-C7-N4	4.38	128.90	121.82
1	2	319	4AC	O7-C7-N4	4.37	128.89	121.82
1	2	774	OMU	N3-C2-N1	4.35	120.67	114.89
1	2	839	4AC	O7-C7-N4	4.34	128.84	121.82
1	2	379	4AC	O7-C7-N4	4.33	128.82	121.82
1	2	1147	4AC	O7-C7-N4	4.28	128.74	121.82
1	2	546	4AC	O7-C7-N4	4.27	128.73	121.82
1	2	511	4AC	O7-C7-N4	4.24	128.68	121.82
1	2	20	OMU	N3-C2-N1	4.24	120.52	114.89
1	2	828	4AC	O7-C7-N4	4.24	128.68	121.82
1	2	626	4AC	O7-C7-N4	4.23	128.67	121.82
1	2	851	4AC	O7-C7-N4	4.22	128.65	121.82
1	2	1177	OMU	N3-C2-N1	4.14	120.39	114.89
1	2	53	4AC	O7-C7-N4	4.12	128.49	121.82
1	2	64	OMU	N3-C2-N1	4.12	120.36	114.89
1	2	394	4AC	O7-C7-N4	4.09	128.44	121.82
1	2	868	4AC	O7-C7-N4	4.07	128.40	121.82
1	2	1469	6MZ	C4-C5-N7	-4.07	105.16	109.40
1	2	751	4AC	O7-C7-N4	4.04	128.35	121.82
1	2	731	4AC	O7-C7-N4	3.91	128.15	121.82
1	2	1479	4AC	O7-C7-N4	3.88	128.10	121.82
1	2	718	4AC	O7-C7-N4	3.84	128.03	121.82
1	2	17	4AC	O7-C7-N4	3.83	128.02	121.82
1	2	636	4AC	N4-C4-N3	3.81	120.25	113.85
1	2	1487	MA6	N3-C2-N1	-3.75	122.82	128.68
1	2	64	OMU	C5-C4-N3	3.75	120.45	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	636	4AC	C5-C4-N4	-3.71	116.48	122.92
1	2	1177	OMU	C5-C4-N3	3.69	120.36	114.84
1	2	1488	MA6	C4-C5-N7	-3.68	105.56	109.40
1	2	830	OMU	C5-C4-N3	3.67	120.33	114.84
1	2	535	5MC	C5-C6-N1	-3.63	119.60	123.34
1	2	1380	OMU	C5-C4-N3	3.59	120.22	114.84
1	2	703	4AC	CM7-C7-N4	-3.59	109.08	115.29
1	2	875	5MC	C5-C6-N1	-3.57	119.67	123.34
1	2	1496	5MC	C5-C6-N1	-3.57	119.67	123.34
1	2	787	OMU	C5-C4-N3	3.54	120.14	114.84
1	2	1469	6MZ	N3-C2-N1	-3.53	123.16	128.68
1	2	1025	5MC	C5-C6-N1	-3.53	119.71	123.34
1	2	1488	MA6	N3-C2-N1	-3.51	123.19	128.68
1	2	20	OMU	C5-C4-N3	3.48	120.05	114.84
1	2	774	OMU	C5-C4-N3	3.47	120.03	114.84
1	2	1505	5MC	C5-C6-N1	-3.42	119.82	123.34
1	2	848	4AC	N4-C4-N3	3.37	119.51	113.85
1	2	1487	MA6	C4-C5-N7	-3.36	105.90	109.40
1	2	1498	5MC	C5-C4-N3	-3.35	118.06	121.67
1	2	373	A2M	N3-C2-N1	-3.31	123.51	128.68
1	2	703	4AC	C5-C4-N4	-3.30	117.18	122.92
1	2	64	OMU	O4-C4-C5	-3.24	119.47	125.16
1	2	1202	5MC	C5-C6-N1	-3.23	120.02	123.34
1	2	828	4AC	CM7-C7-N4	-3.13	109.88	115.29
1	2	373	A2M	C4-C5-N7	-3.07	106.19	109.40
1	2	479	4AC	N4-C4-N3	3.05	118.98	113.85
1	2	839	4AC	N4-C4-N3	3.00	118.89	113.85
1	2	1147	4AC	N4-C4-N3	2.98	118.86	113.85
1	2	303	4AC	CM7-C7-N4	-2.97	110.15	115.29
1	2	774	OMU	O4-C4-C5	-2.97	119.93	125.16
1	2	830	OMU	O4-C4-C5	-2.89	120.09	125.16
1	2	1233	4AC	N4-C4-N3	2.88	118.69	113.85
1	2	1374	5MC	C5-C4-N3	-2.87	118.58	121.67
1	2	693	5MC	C5-C6-N1	-2.85	120.40	123.34
1	2	1374	5MC	C5-C6-N1	-2.83	120.42	123.34
1	2	379	4AC	CM7-C7-N4	-2.81	110.43	115.29
1	2	1147	4AC	C5-C4-N4	-2.81	118.04	122.92
1	2	1184	4AC	C5-C4-N4	-2.80	118.05	122.92
1	2	1233	4AC	CM7-C7-N4	-2.79	110.47	115.29
1	2	626	4AC	N4-C4-N3	2.78	118.52	113.85
1	2	535	5MC	C5-C4-N3	-2.75	118.70	121.67
1	2	773	OMC	O2-C2-N3	-2.74	117.87	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	703	4AC	N4-C4-N3	2.74	118.45	113.85
1	2	319	4AC	N4-C4-N3	2.74	118.45	113.85
1	2	20	OMU	O4-C4-C5	-2.74	120.34	125.16
1	2	1496	5MC	C5-C4-N3	-2.74	118.72	121.67
1	2	590	4AC	CM7-C7-N4	-2.73	110.56	115.29
1	2	848	4AC	C5-C4-N4	-2.73	118.18	122.92
1	2	957	4AC	CM7-C7-N4	-2.72	110.58	115.29
1	2	1184	4AC	N4-C4-N3	2.71	118.41	113.85
1	2	1380	OMU	O4-C4-C5	-2.71	120.39	125.16
1	2	1184	4AC	CM7-C7-N4	-2.71	110.60	115.29
1	2	286	4AC	CM7-C7-N4	-2.71	110.61	115.29
1	2	394	4AC	N4-C4-N3	2.70	118.39	113.85
1	2	546	4AC	CM7-C7-N4	-2.70	110.63	115.29
1	2	1025	5MC	C5-C4-N3	-2.70	118.77	121.67
1	2	1202	5MC	C5-C4-N3	-2.69	118.77	121.67
1	2	1505	5MC	C5-C4-N3	-2.69	118.77	121.67
1	2	787	OMU	O4-C4-C5	-2.68	120.45	125.16
1	2	1041	LHH	C5-C4-N3	-2.66	118.30	122.59
1	2	1498	5MC	O2-C2-N3	-2.65	118.02	122.33
1	2	1028	4AC	N4-C4-N3	2.65	118.31	113.85
1	2	479	4AC	CM7-C7-N4	-2.65	110.71	115.29
1	2	479	4AC	C5-C4-N4	-2.64	118.33	122.92
1	2	511	4AC	CM7-C7-N4	-2.64	110.72	115.29
1	2	250	LHH	C5-C4-N3	-2.64	118.35	122.59
1	2	1233	4AC	C5-C4-N4	-2.63	118.35	122.92
1	2	1028	4AC	CM7-C7-N4	-2.63	110.75	115.29
1	2	1239	4AC	CM7-C7-N4	-2.62	110.75	115.29
1	2	693	5MC	C5-C4-N3	-2.62	118.84	121.67
1	2	934	OMG	C8-N7-C5	2.62	107.98	102.99
31	4	32	OMC	O2-C2-N3	-2.62	118.08	122.33
1	2	839	4AC	CM7-C7-N4	-2.61	110.78	115.29
1	2	286	4AC	N4-C4-N3	2.60	118.22	113.85
1	2	787	OMU	O2-C2-N1	-2.59	119.34	122.79
1	2	53	4AC	N4-C4-N3	2.59	118.20	113.85
1	2	519	OMG	C5-C6-N1	2.58	118.51	113.95
1	2	913	OMG	C5-C6-N1	2.58	118.50	113.95
1	2	718	4AC	N4-C4-N3	2.55	118.14	113.85
1	2	913	OMG	C8-N7-C5	2.55	107.84	102.99
1	2	839	4AC	C5-C4-N4	-2.52	118.54	122.92
1	2	1147	4AC	CM7-C7-N4	-2.52	110.94	115.29
1	2	1479	4AC	O2-C2-N3	-2.52	118.24	122.33
1	2	751	4AC	CM7-C7-N4	-2.51	110.95	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1467	UR3	C6-N1-C2	-2.50	119.55	121.79
1	2	394	4AC	CM7-C7-N4	-2.50	110.96	115.29
1	2	467	OMG	C8-N7-C5	2.50	107.75	102.99
1	2	286	4AC	C5-C4-N4	-2.50	118.58	122.92
1	2	731	4AC	N4-C4-N3	2.49	118.04	113.85
1	2	938	B8H	N3-C2-N1	2.48	117.82	115.14
1	2	851	4AC	CM7-C7-N4	-2.48	111.01	115.29
1	2	875	5MC	C5-C4-N3	-2.47	119.01	121.67
1	2	1496	5MC	O2-C2-N3	-2.47	118.31	122.33
1	2	1177	OMU	O4-C4-C5	-2.46	120.83	125.16
1	2	250	LHH	N4-C4-N3	2.45	117.96	113.85
1	2	394	4AC	C5-C4-N4	-2.44	118.68	122.92
1	2	636	4AC	CM7-C7-N4	-2.43	111.08	115.29
1	2	1069	OMG	C8-N7-C5	2.43	107.62	102.99
1	2	751	4AC	N4-C4-N3	2.43	117.93	113.85
1	2	1028	4AC	C5-C4-N4	-2.42	118.71	122.92
1	2	868	4AC	CM7-C7-N4	-2.42	111.11	115.29
1	2	873	OMG	C8-N7-C5	2.41	107.59	102.99
1	2	1380	OMU	O2-C2-N1	-2.41	119.58	122.79
1	2	471	OMG	C5-C6-N1	2.41	118.20	113.95
1	2	680	OMG	C8-N7-C5	2.40	107.56	102.99
1	2	319	4AC	CM7-C7-N4	-2.39	111.15	115.29
1	2	53	4AC	C5-C4-N4	-2.38	118.78	122.92
1	2	17	4AC	N4-C4-N3	2.38	117.85	113.85
1	2	1239	4AC	N4-C4-N3	2.38	117.85	113.85
1	2	1036	OMC	O2-C2-N3	-2.37	118.48	122.33
1	2	680	OMG	C5-C6-N1	2.36	118.13	113.95
1	2	957	4AC	N4-C4-N3	2.36	117.82	113.85
1	2	626	4AC	CM7-C7-N4	-2.36	111.22	115.29
1	2	471	OMG	C8-N7-C5	2.35	107.47	102.99
1	2	868	4AC	N4-C4-N3	2.35	117.79	113.85
1	2	1041	LHH	N4-C4-N3	2.34	117.78	113.85
1	2	934	OMG	C5-C6-N1	2.34	118.08	113.95
1	2	250	LHH	O2-C2-N3	-2.34	118.53	122.33
1	2	1374	5MC	O2-C2-N3	-2.33	118.54	122.33
1	2	53	4AC	CM7-C7-N4	-2.32	111.27	115.29
1	2	1498	5MC	C1'-N1-C6	-2.32	117.26	121.12
1	2	467	OMG	C5-C6-N1	2.31	118.03	113.95
1	2	1479	4AC	N4-C4-N3	2.29	117.70	113.85
1	2	693	5MC	O2-C2-N3	-2.29	118.61	122.33
1	2	657	OMG	C8-N7-C5	2.29	107.35	102.99
1	2	590	4AC	N4-C4-N3	2.28	117.68	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	535	5MC	O2-C2-N3	-2.28	118.62	122.33
1	2	657	OMG	C5-C6-N1	2.28	117.98	113.95
1	2	303	4AC	N4-C4-N3	2.27	117.66	113.85
1	2	519	OMG	C8-N7-C5	2.26	107.29	102.99
1	2	873	OMG	C5-C6-N1	2.25	117.92	113.95
1	2	1498	5MC	C1'-N1-C2	2.25	123.44	118.42
1	2	1487	MA6	N1-C6-N6	2.25	119.42	117.06
1	2	1505	5MC	O2-C2-N3	-2.24	118.69	122.33
1	2	848	4AC	CM7-C7-N4	-2.24	111.42	115.29
1	2	828	4AC	N4-C4-N3	2.24	117.61	113.85
1	2	319	4AC	C5-C4-N4	-2.23	119.04	122.92
1	2	1041	LHH	O2-C2-N3	-2.23	118.71	122.33
1	2	957	4AC	C5-C4-N4	-2.22	119.05	122.92
1	2	20	OMU	O2-C2-N1	-2.22	119.83	122.79
1	2	626	4AC	C5-C4-N4	-2.17	119.15	122.92
1	2	546	4AC	N4-C4-N3	2.16	117.49	113.85
1	2	851	4AC	O2-C2-N3	-2.16	118.82	122.33
31	4	32	OMC	C1'-N1-C2	2.15	123.22	118.42
1	2	535	5MC	CM5-C5-C6	-2.14	119.99	122.85
1	2	1202	5MC	O2-C2-N3	-2.14	118.86	122.33
1	2	1069	OMG	C5-C6-N1	2.14	117.72	113.95
1	2	379	4AC	O2-C2-N3	-2.13	118.86	122.33
1	2	938	B8H	O4'-C1'-C2'	2.13	108.15	105.14
1	2	511	4AC	O2-C2-N3	-2.13	118.87	122.33
1	2	1041	LHH	C5-C6-N1	-2.12	118.25	121.81
1	2	511	4AC	N4-C4-N3	2.12	117.42	113.85
1	2	1498	5MC	C5-C6-N1	-2.12	121.16	123.34
1	2	718	4AC	O2-C2-N3	-2.11	118.90	122.33
1	2	731	4AC	CM7-C7-N4	-2.11	111.65	115.29
1	2	17	4AC	O2-C2-N3	-2.11	118.90	122.33
1	2	590	4AC	C5-C4-N4	-2.10	119.28	122.92
1	2	828	4AC	C5-C4-N4	-2.10	119.28	122.92
1	2	250	LHH	C5-C6-N1	-2.09	118.32	121.81
1	2	846	OMC	O2-C2-N3	-2.08	118.95	122.33
1	2	17	4AC	CM7-C7-N4	-2.08	111.69	115.29
1	2	751	4AC	C5-C4-N4	-2.08	119.31	122.92
1	2	718	4AC	C5-C4-N4	-2.07	119.32	122.92
1	2	718	4AC	CM7-C7-N4	-2.06	111.73	115.29
1	2	1239	4AC	C5-C4-N4	-2.04	119.37	122.92
1	2	875	5MC	O2-C2-N3	-2.03	119.03	122.33
1	2	1025	5MC	O2-C2-N3	-2.00	119.07	122.33

There are no chirality outliers.



All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1202	5MC	O4'-C4'-C5'-O5'
1	2	20	OMU	C2'-C1'-N1-C6
31	4	32	OMC	C3'-C2'-O2'-CM2
1	2	20	OMU	O4'-C1'-N1-C6
1	2	1202	5MC	C3'-C4'-C5'-O5'
1	2	787	OMU	C2'-C1'-N1-C6
1	2	1498	5MC	O4'-C1'-N1-C6
1	2	1488	MA6	C4'-C5'-O5'-P
1	2	20	OMU	O4'-C1'-N1-C2
1	2	787	OMU	O4'-C1'-N1-C6
1	2	1498	5MC	O4'-C1'-N1-C2
1	2	1498	5MC	O4'-C4'-C5'-O5'
1	2	1498	5MC	C2'-C1'-N1-C2
1	2	20	OMU	C2'-C1'-N1-C2
1	2	787	OMU	O4'-C1'-N1-C2
31	4	32	OMC	C2'-C1'-N1-C2
1	2	787	OMU	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 4.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 96 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 4.7 Other polymers

There are no such residues in this entry.

## 4.8 Polymer linkage issues

There are no chain breaks in this entry.

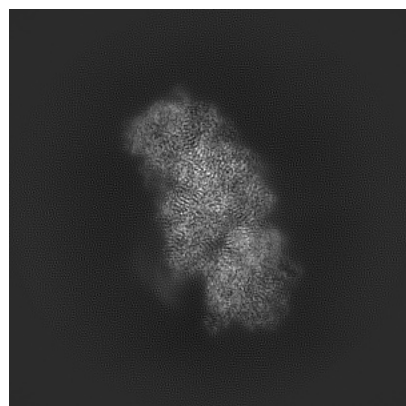
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14731. These allow visual inspection of the internal detail of the map and identification of artifacts.

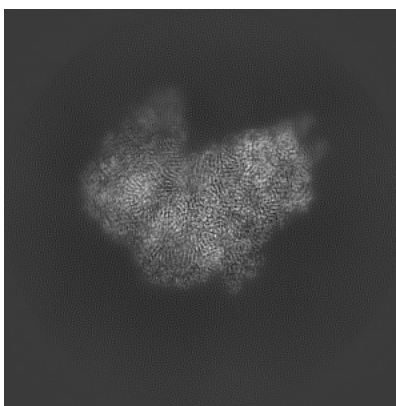
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

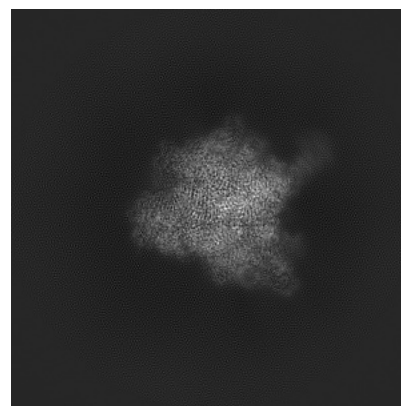
#### 5.1.1 Primary map



X

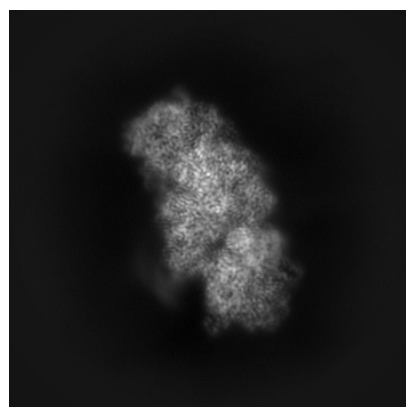


Y

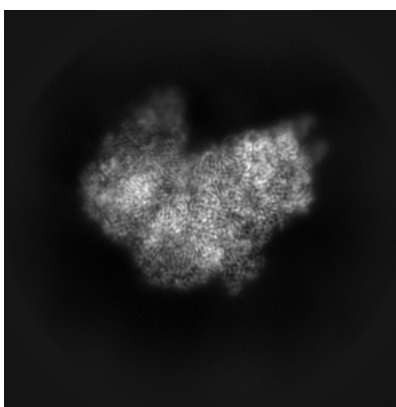


Z

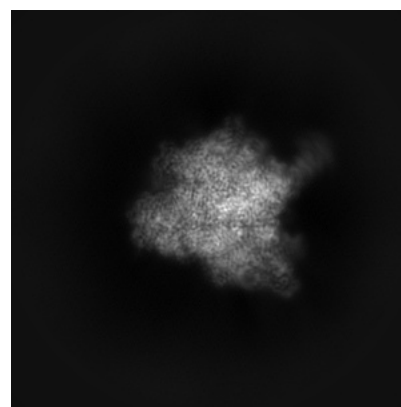
#### 5.1.2 Raw map



X



Y

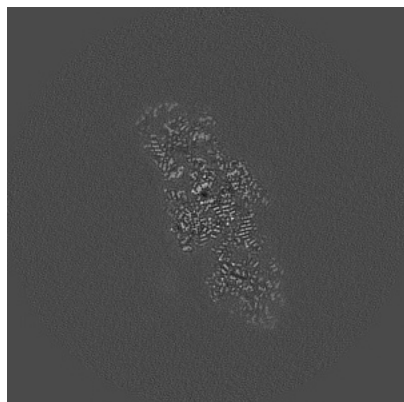


Z

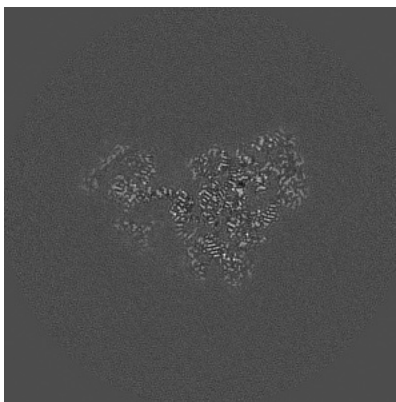
The images above show the map projected in three orthogonal directions.

## 5.2 Central slices [i](#)

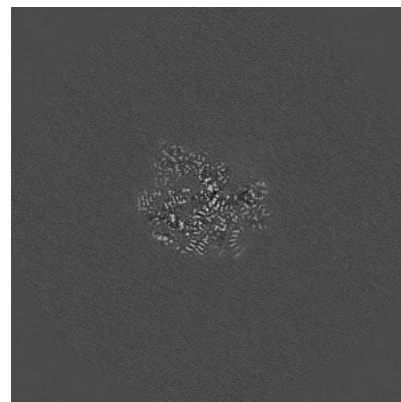
### 5.2.1 Primary map



X Index: 216

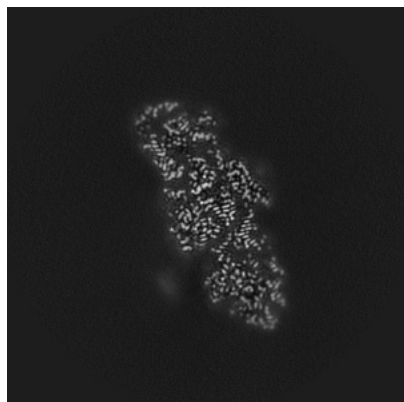


Y Index: 216

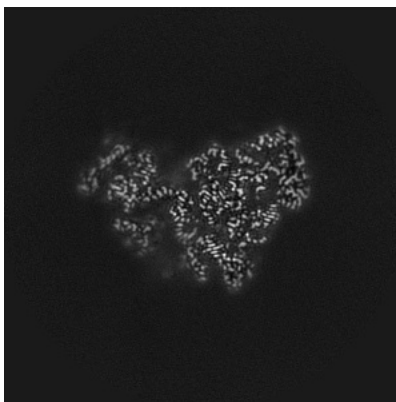


Z Index: 216

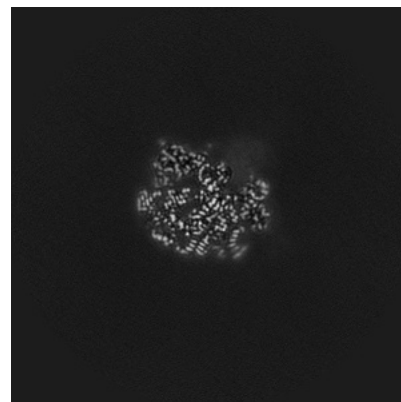
### 5.2.2 Raw map



X Index: 216



Y Index: 216

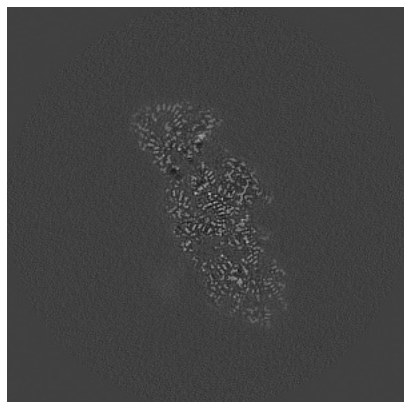


Z Index: 216

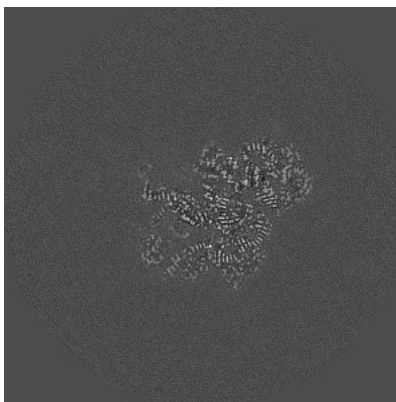
The images above show central slices of the map in three orthogonal directions.

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

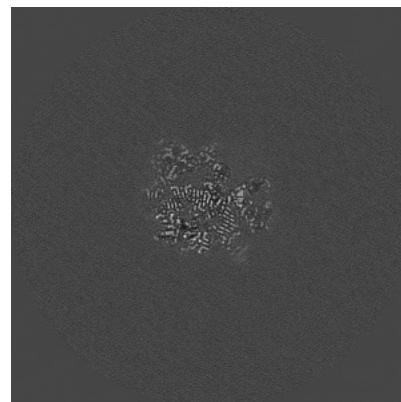
### 5.3.1 Primary map



X Index: 221

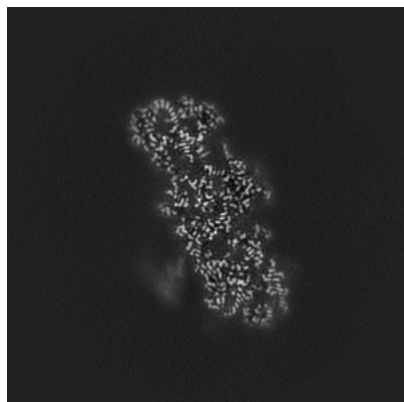


Y Index: 207

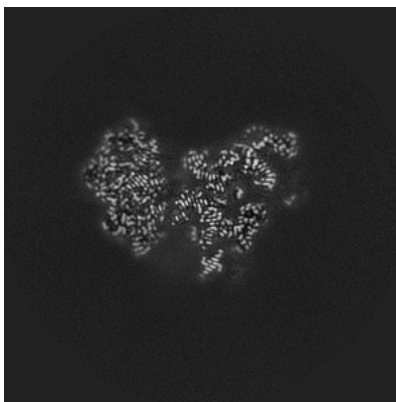


Z Index: 222

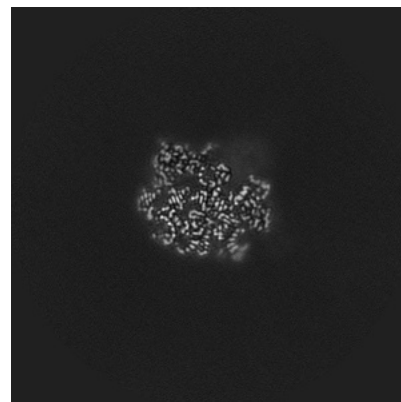
### 5.3.2 Raw map



X Index: 225



Y Index: 229

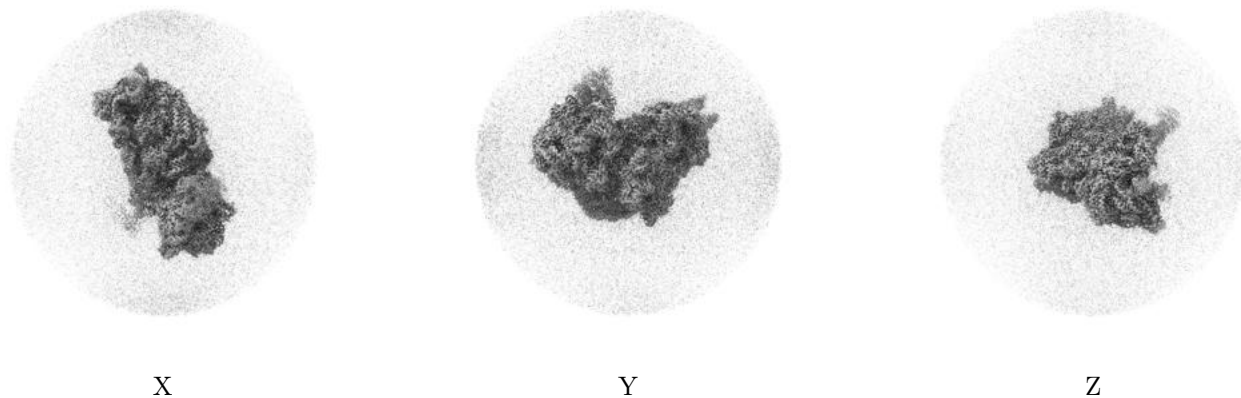


Z Index: 218

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

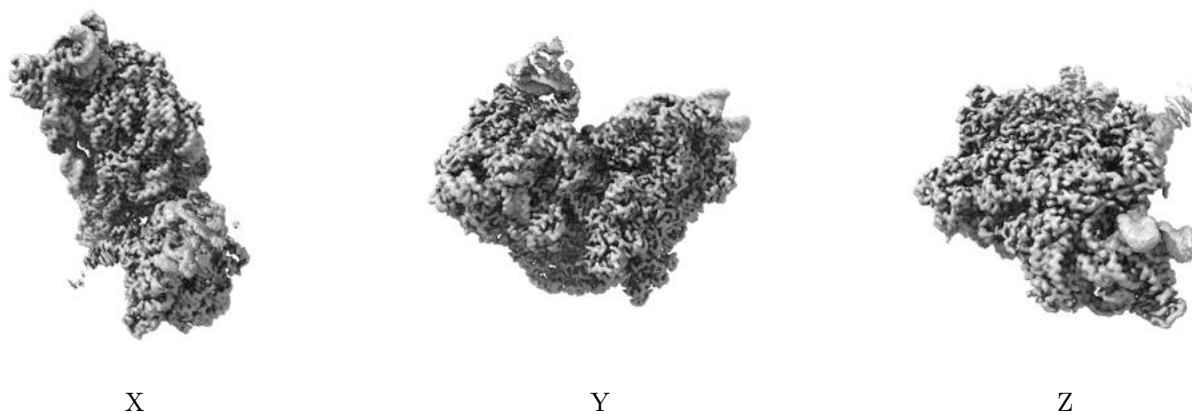
## 5.4 Orthogonal surface views [i](#)

### 5.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0249. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 5.4.2 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.

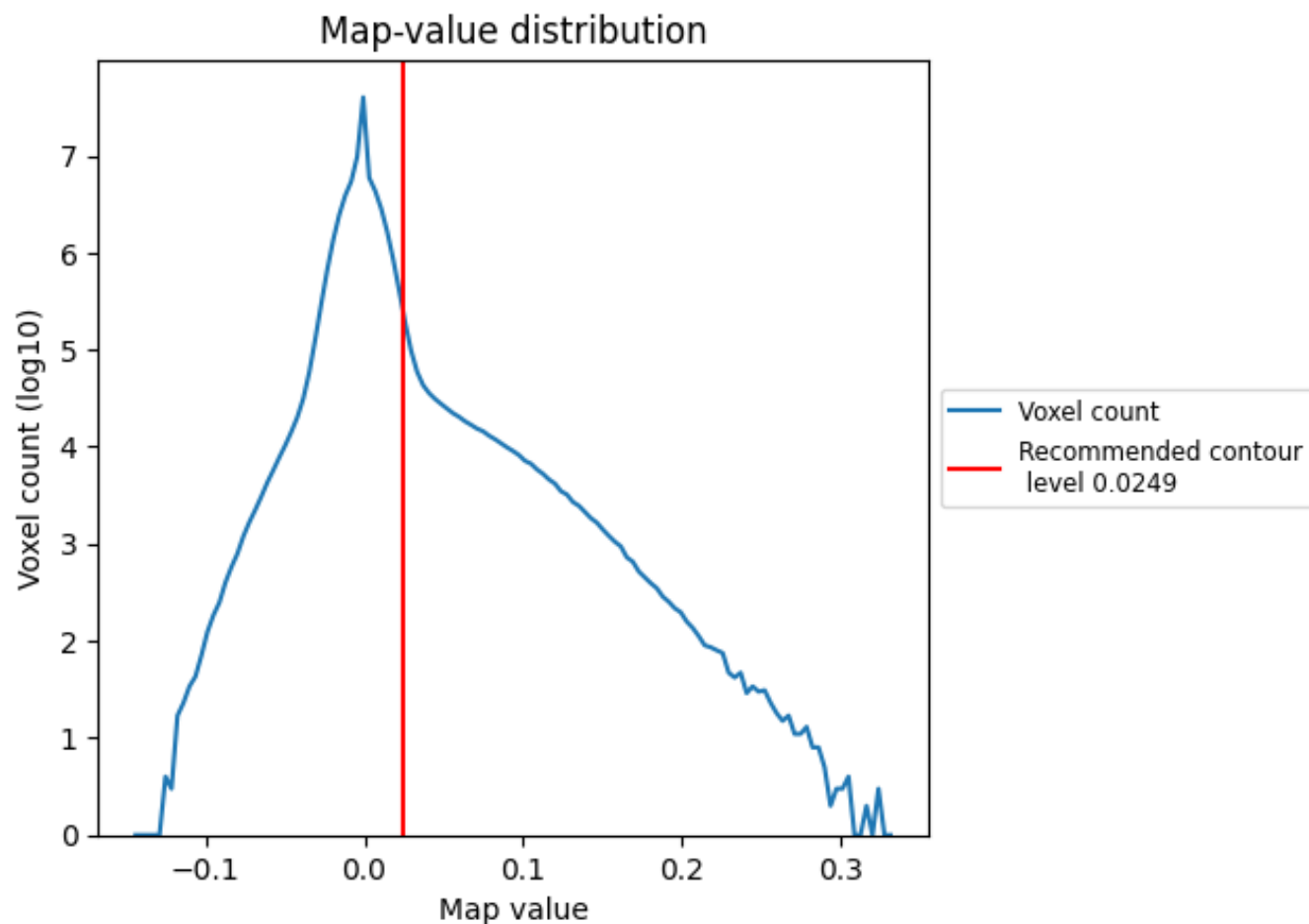
## 5.5 Mask visualisation [i](#)

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

## 6 Map analysis [i](#)

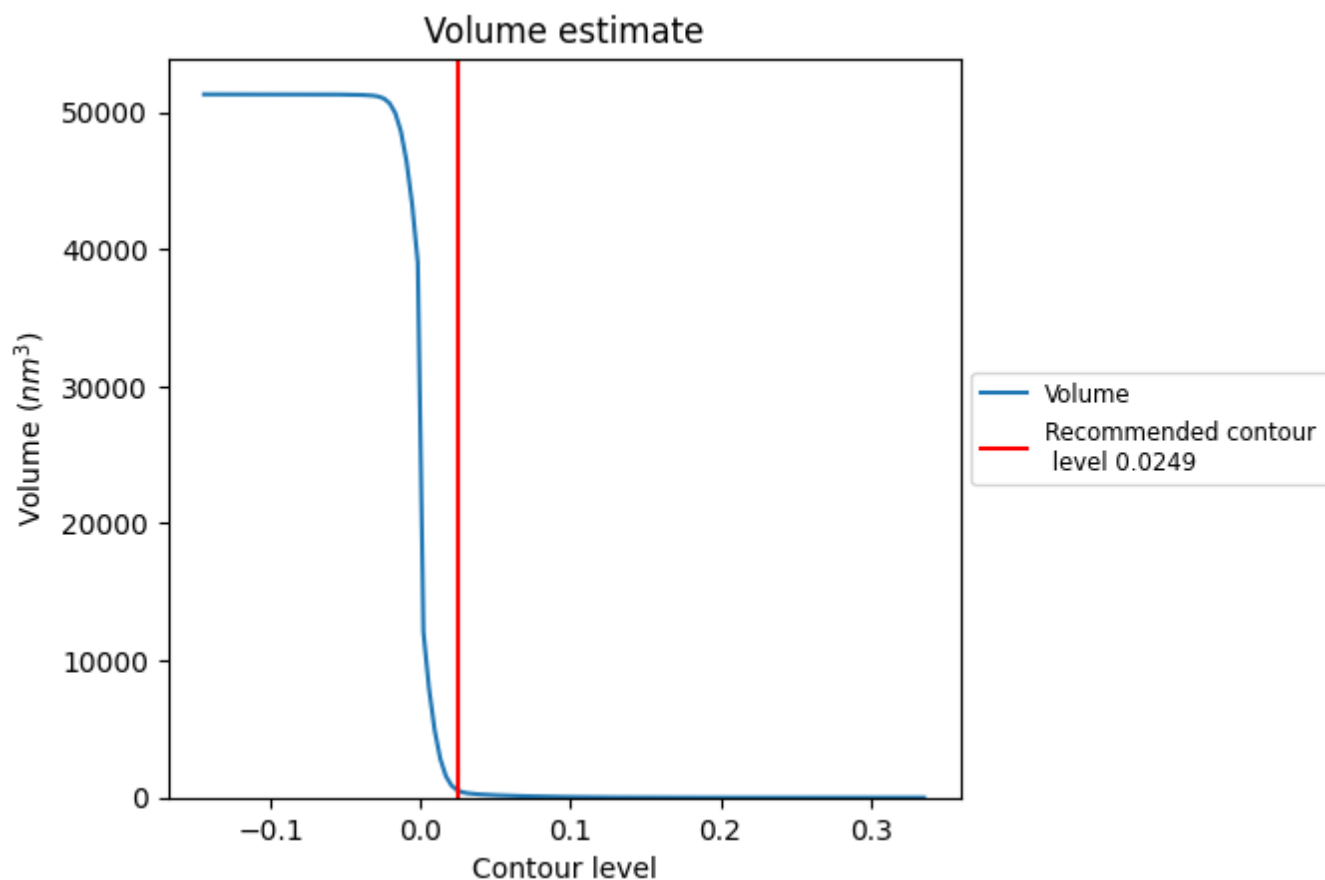
This section contains the results of statistical analysis of the map.

### 6.1 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.

## 6.2 Volume estimate [i](#)

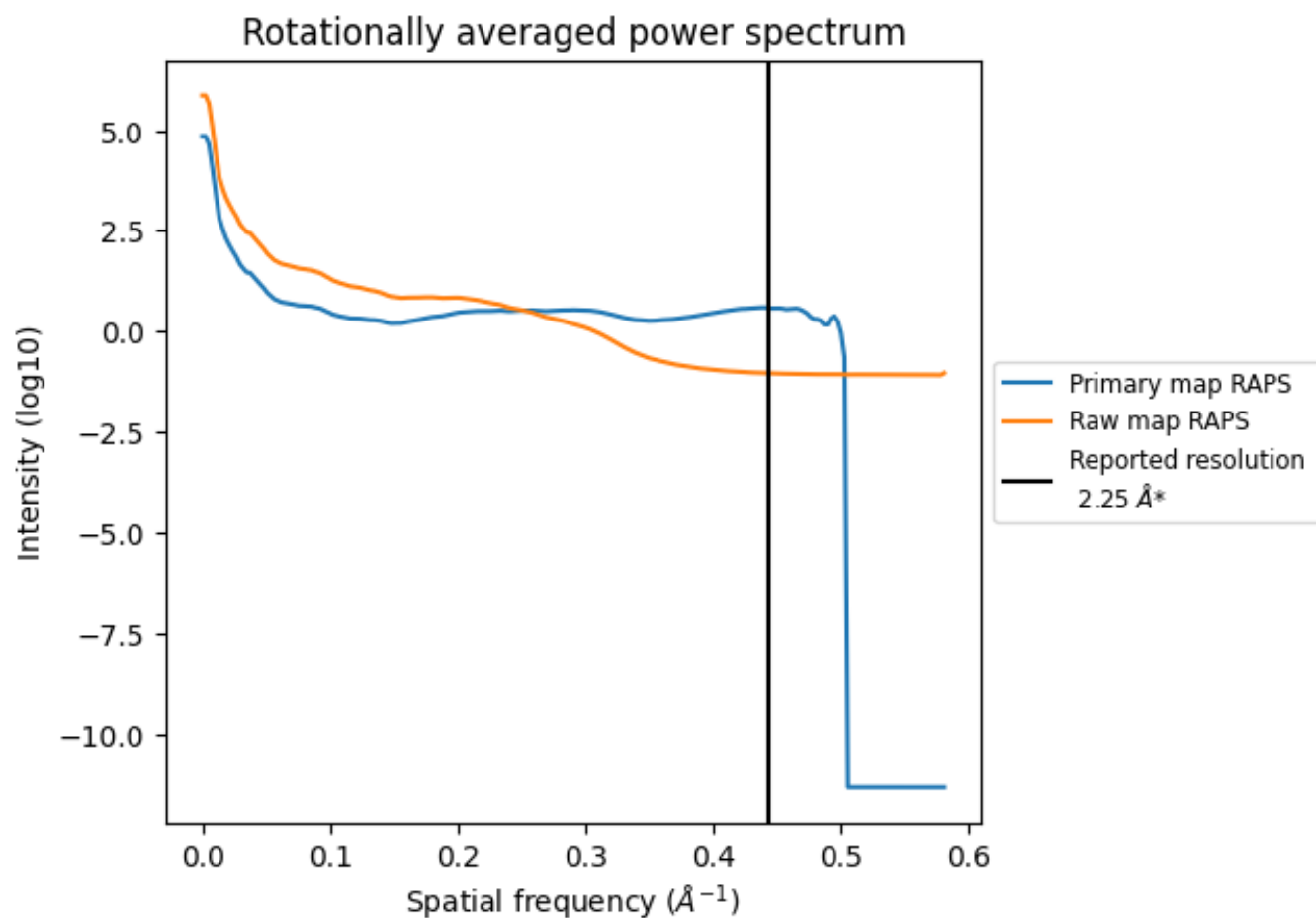


The volume at the recommended contour level is 521 nm<sup>3</sup>; this corresponds to an approximate mass of 470 kDa.

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.



### 6.3 Rotationally averaged power spectrum ⓘ

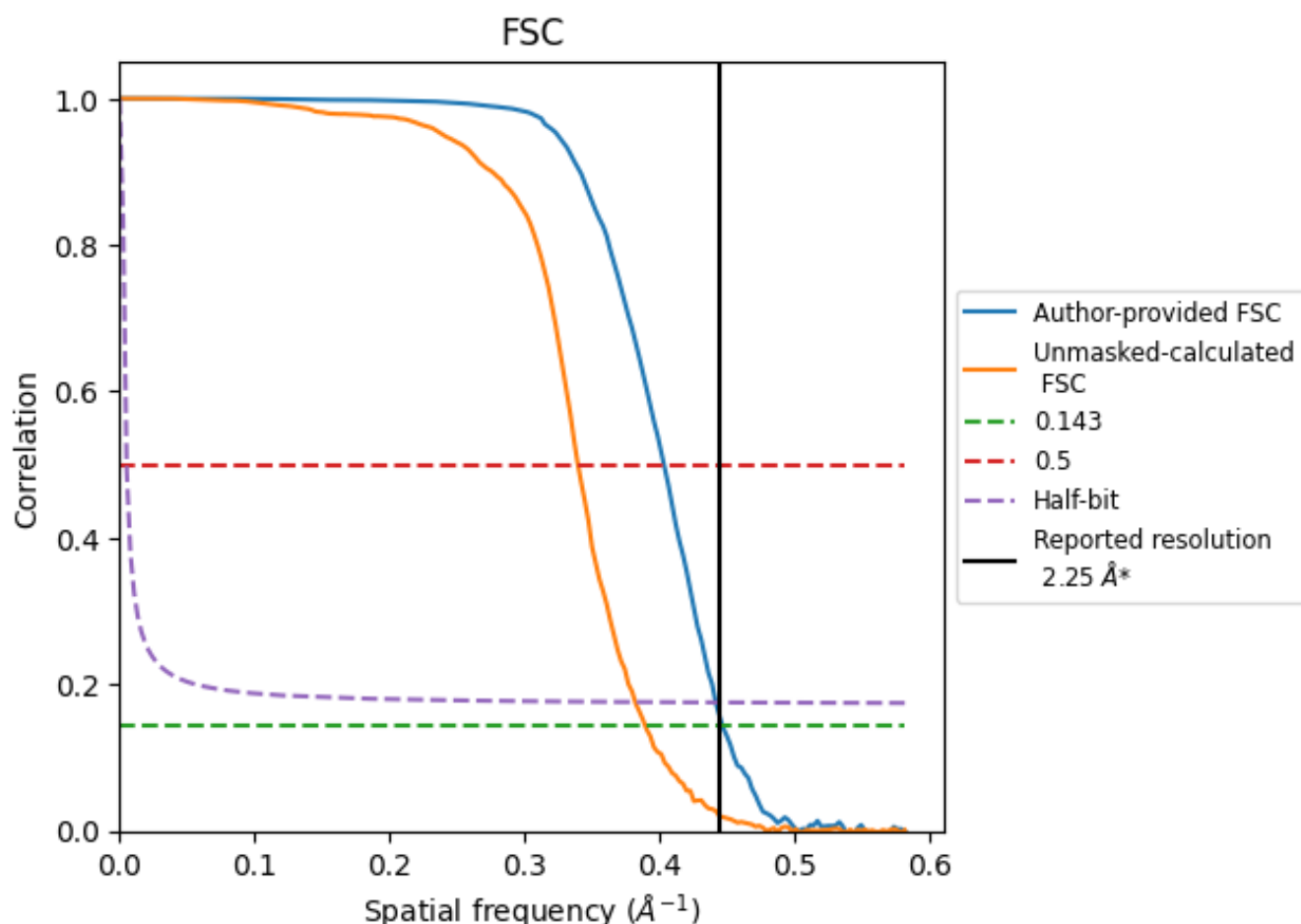


\*Reported resolution corresponds to spatial frequency of 0.444 Å<sup>-1</sup>

## 7 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.

### 7.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.444 Å<sup>-1</sup>

## 7.2 Resolution estimates [i](#)

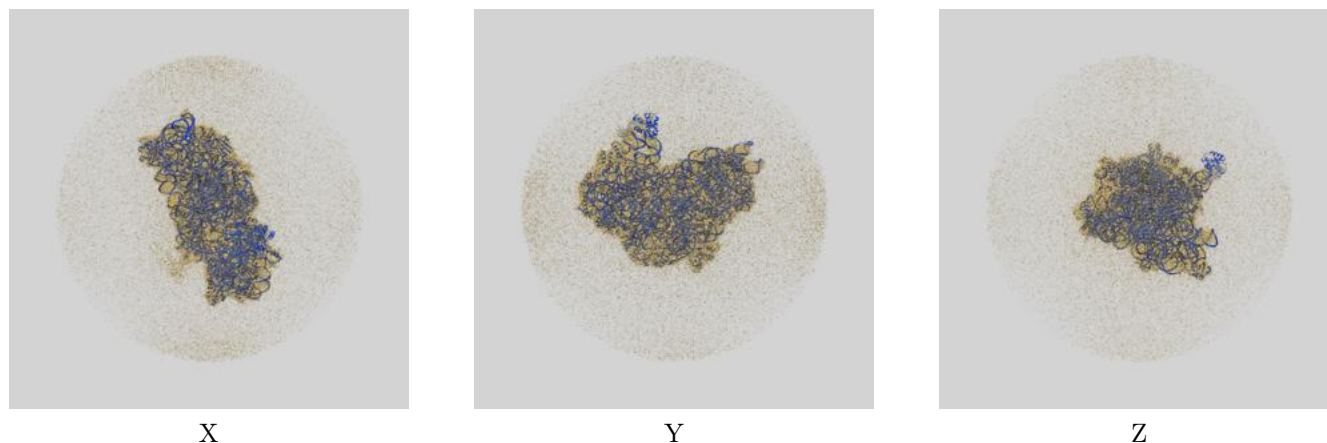
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.24	2.48	2.27
Unmasked-calculated*	2.57	2.95	2.62

\*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 2.57 differs from the reported value 2.25 by more than 10 %

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

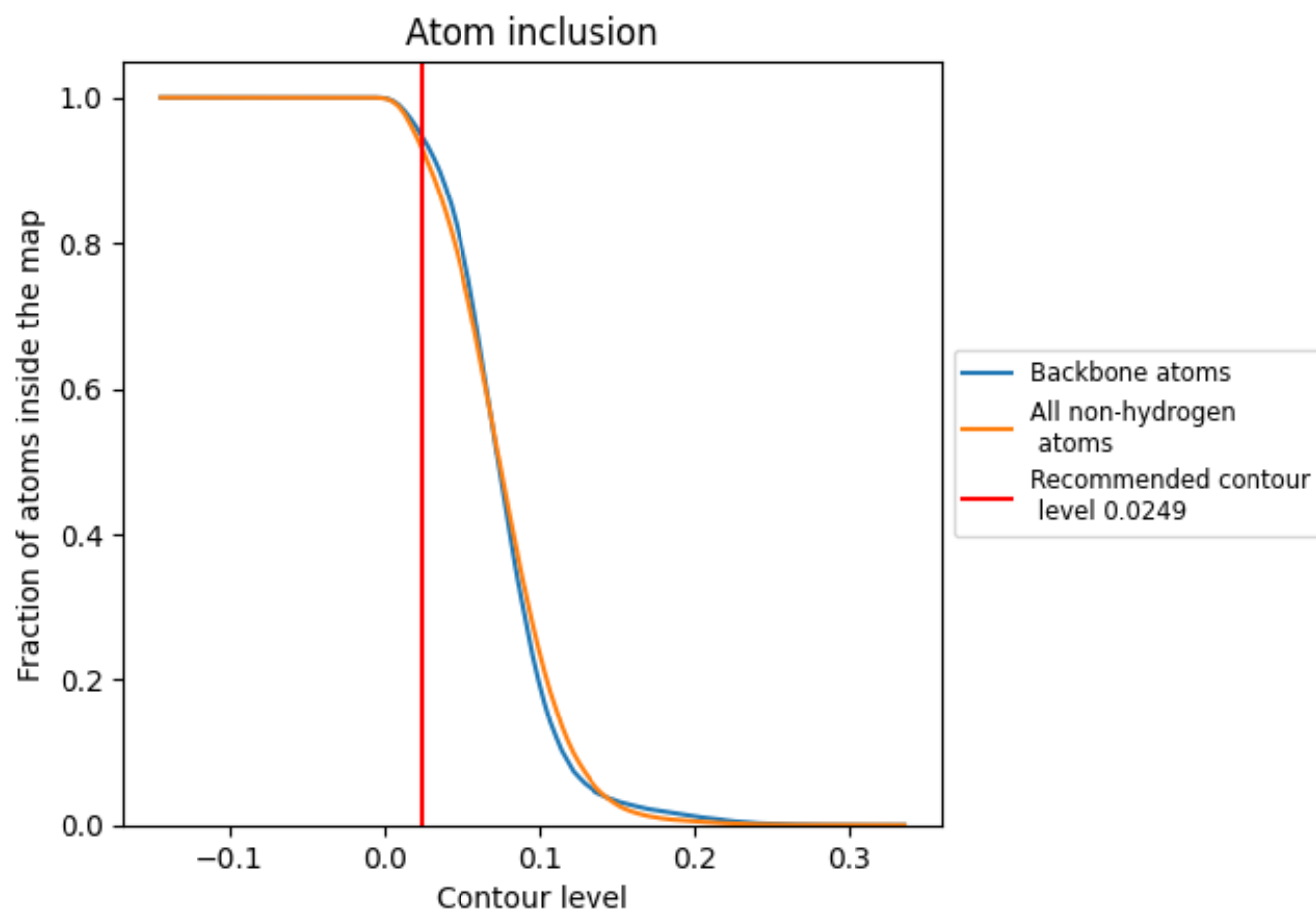
This section contains information regarding the fit between EMDB map EMD-14731 and PDB model 7ZHG. Per-residue inclusion information can be found in section ?? on page ??.

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



The images above show the 3D surface view of the map at the recommended contour level 0.0249 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.

## 8.2 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.