Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 04:47 pm GMT

PDB ID	:	6YS3
EMDB ID	:	EMD-10891
Title	:	Cryo-EM structure of the 50S ribosomal subunit at 2.58 Angstroms with modeled GBC SecM peptide
Authors	:	Schulte, L.; Reitz, J.; Kudlinzki, D.; Hodirnau, V.V.; Frangakis, A.; Schwalbe, H.
Deposited on	:	2020-04-20
Resolution	:	2.58 Å(reported)
Based on initial model	:	3JBU

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:

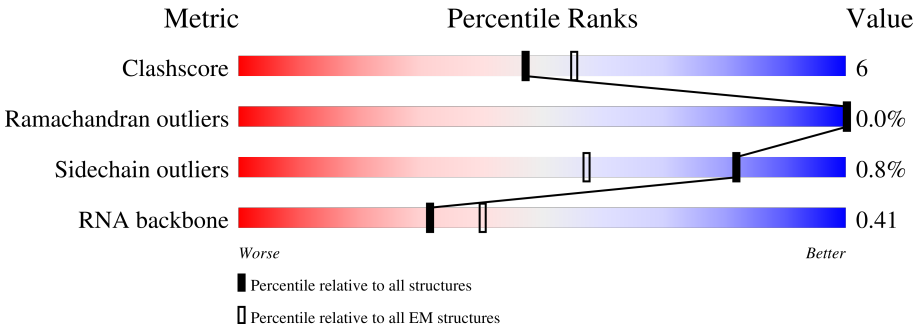
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.58 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.



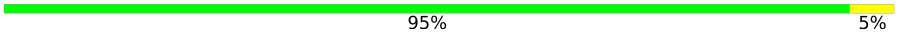
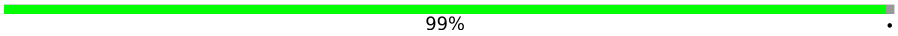
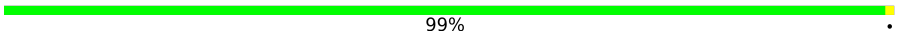
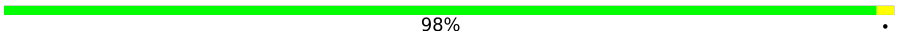
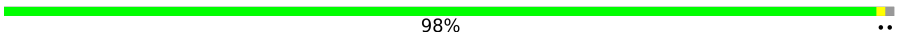
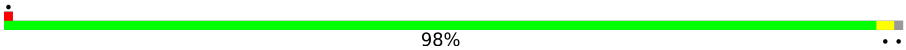
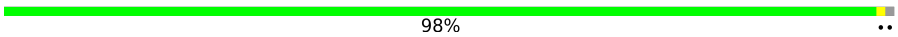
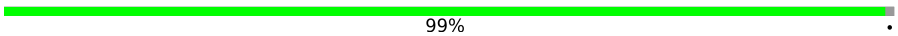
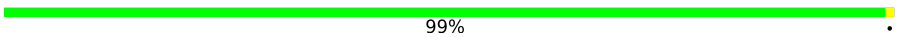
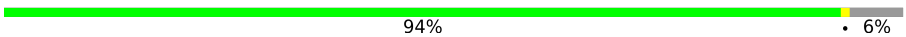
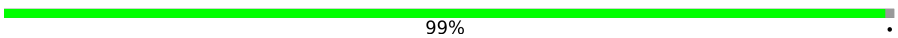
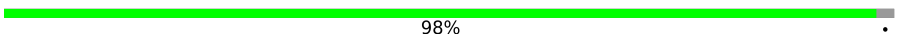
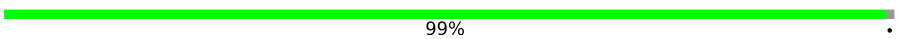
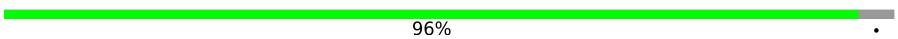
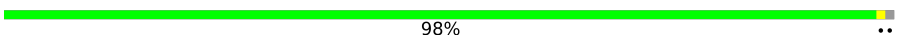
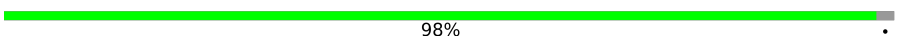
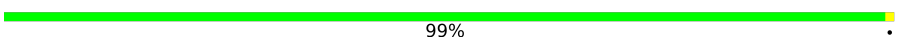
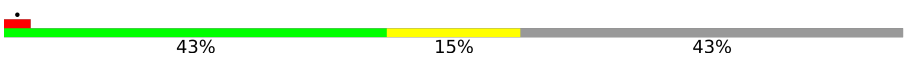
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	0	78	92% 6% •
2	1	63	83% 14% •
3	2	59	93% • •
4	3	57	84% 12% •
5	4	55	84% 7% 9%
6	6	46	96% •
7	7	65	92% • • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	8	38	
9	a	120	
10	b	2906	
11	c	273	
12	d	209	
13	e	201	
14	f	179	
15	g	177	
16	h	149	
17	j	142	
18	k	123	
19	l	144	
20	m	136	
21	n	127	
22	o	117	
23	p	115	
24	q	118	
25	r	103	
26	s	110	
27	t	100	
28	u	104	
29	v	75	
30	w	94	
31	y	85	
32	z	61	

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 90553 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 protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

- Molecule 4 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 5 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 6 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	118	Total	C	N	O	P	0	0
			2528	1126	464	821	117		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	2888	Total	C	N	O	P	0	0
			62008	27660	11413	20047	2888		

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 13 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	39	Total	C	N	O	S	0	0
			287	184	51	51	1		

- Molecule 17 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	j	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	l	143	Total	C	N	O	S	0	0
			1042	648	206	186	2		

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	m	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	o	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	p	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	99	Total	C	N	O	S	0	0
			791	500	149	140	2		

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	t	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	u	102	Total 779	C 492	N 146	O 141	0	0

- Molecule 29 is a RNA chain called glycine-tRNA glyT.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	v	75	Total 1583	C 707	N 270	O 531	P 75	0	0

- Molecule 30 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	w	94	Total 753	C 479	N 137	O 134	S 3	0	0

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	y	74	Total 559	C 348	N 112	O 98	S 1	0	0

- Molecule 32 is a protein called Gamma-crystallin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	z	35	Total 275	C 172	N 48	O 51	S 4	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	-12	MET	-	initiating methionine	UNP P02526
z	-11	GLY	-	expression tag	UNP P02526
z	-10	HIS	-	expression tag	UNP P02526
z	-9	HIS	-	expression tag	UNP P02526
z	-8	HIS	-	expression tag	UNP P02526
z	-7	HIS	-	expression tag	UNP P02526
z	-6	HIS	-	expression tag	UNP P02526
z	-5	HIS	-	expression tag	UNP P02526
z	-4	HIS	-	expression tag	UNP P02526
z	-3	HIS	-	expression tag	UNP P02526
z	-2	HIS	-	expression tag	UNP P02526
z	-1	HIS	-	expression tag	UNP P02526

Continued on next page...

Continued from previous page...

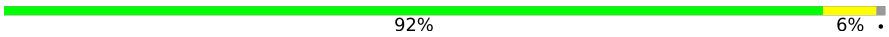
Chain	Residue	Modelled	Actual	Comment	Reference
z	150	PHE	ASN	conflict	UNP P02526
z	152	THR	ILE	conflict	UNP P02526
z	153	PRO	ARG	conflict	UNP P02526
z	155	TRP	-	expression tag	UNP P02526
z	156	ILE	-	expression tag	UNP P02526
z	157	SER	-	expression tag	UNP P02526
z	158	GLN	-	expression tag	UNP P02526
z	159	ALA	-	expression tag	UNP P02526
z	160	GLN	-	expression tag	UNP P02526
z	161	GLY	-	expression tag	UNP P02526
z	162	ILE	-	expression tag	UNP P02526
z	163	ARG	-	expression tag	UNP P02526
z	164	ALA	-	expression tag	UNP P02526
z	165	GLY	-	expression tag	UNP P02526

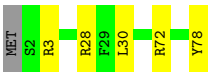
3 Residue-property plots (i)

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: 50S ribosomal protein L28

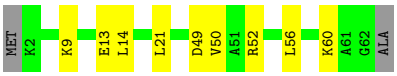
Chain 0:





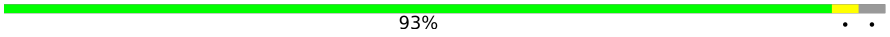
• Molecule 2: 50S ribosomal protein L29

Chain 1:



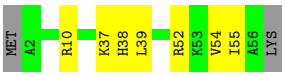
• Molecule 3: 50S ribosomal protein L30

Chain 2:



• Molecule 4: 50S ribosomal protein L32

Chain 3:

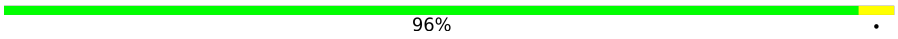


• Molecule 5: 50S ribosomal protein L33

Chain 4:

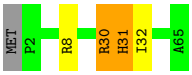
• Molecule 6: 50S ribosomal protein L34

Chain 6:



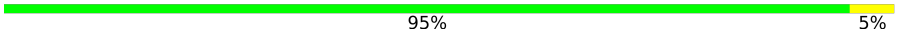
• Molecule 7: 50S ribosomal protein L35

Chain 7:



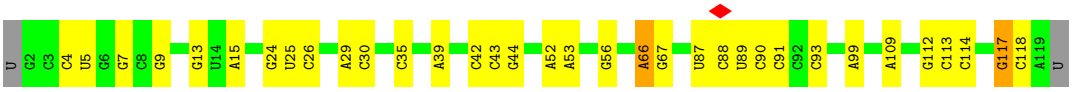
• Molecule 8: 50S ribosomal protein L36

Chain 8:



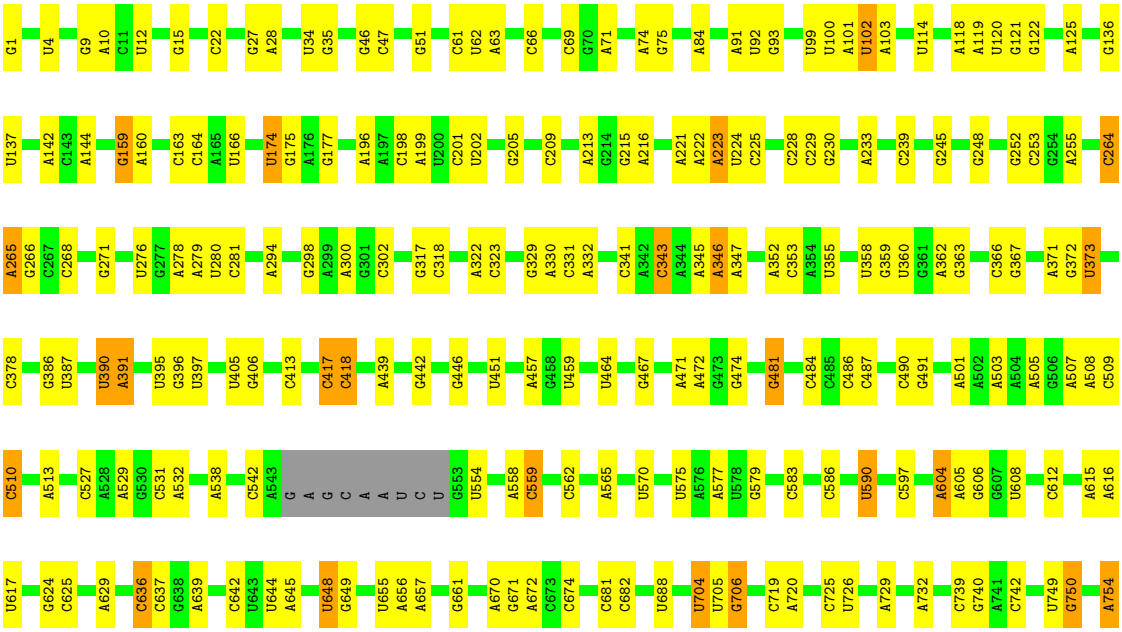
• Molecule 9: 5S rRNA

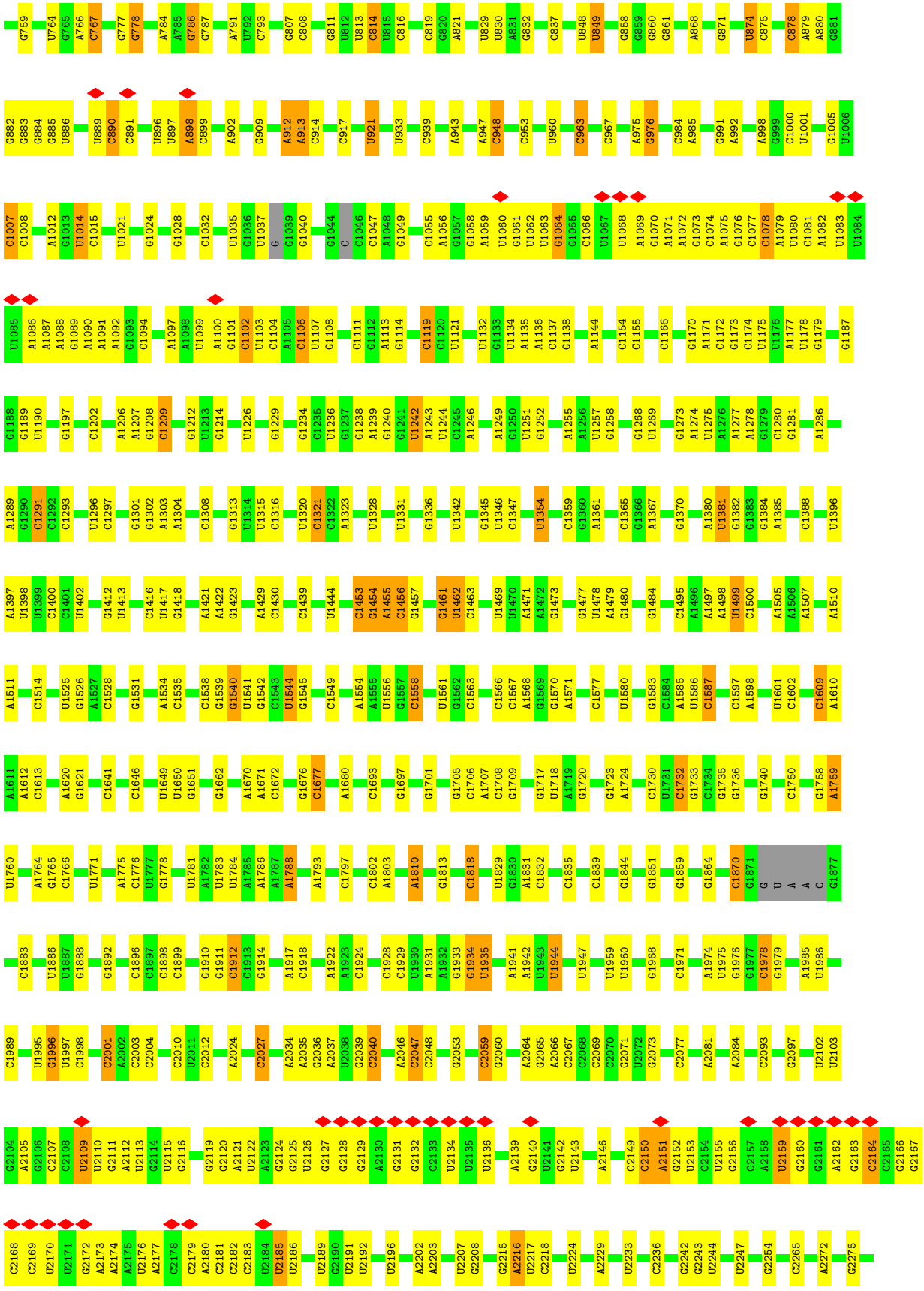
Chain a:

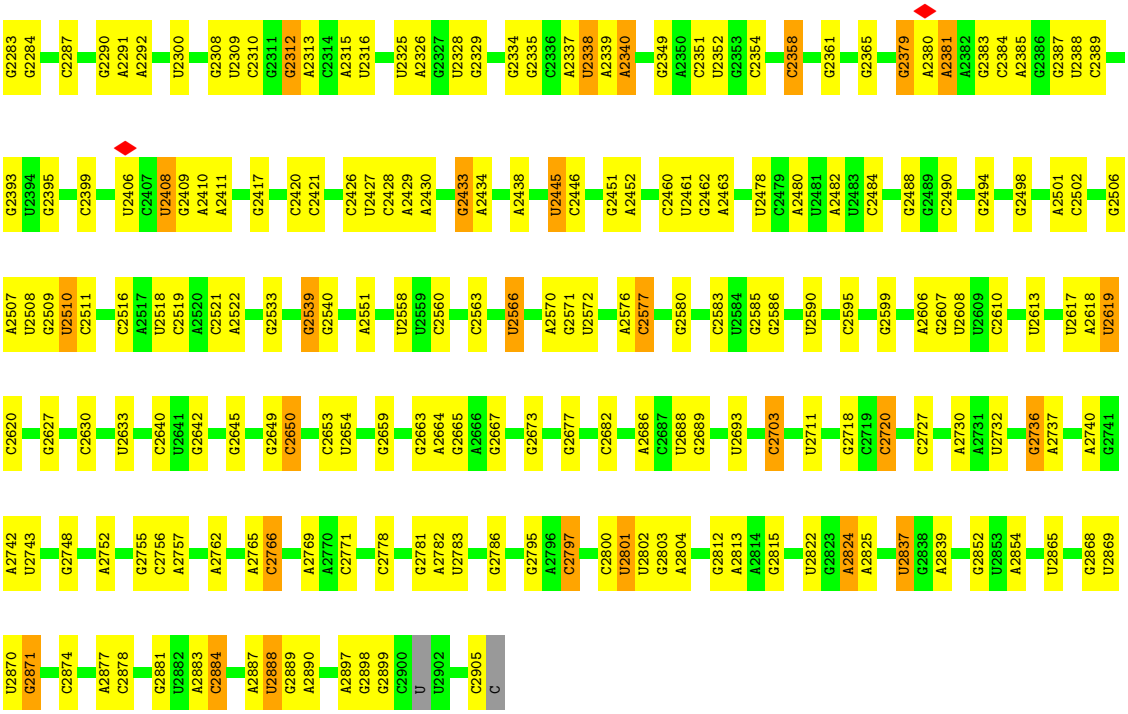


• Molecule 10: 23S rRNA

Chain b:

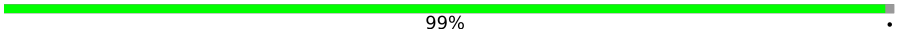






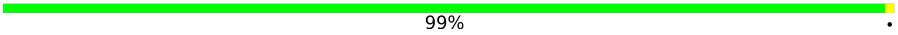
• Molecule 11: 50S ribosomal protein L2

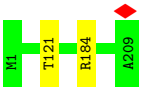
Chain c:



• Molecule 12: 50S ribosomal protein L3

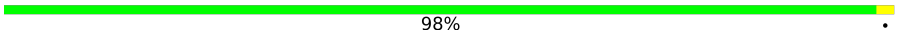
Chain d:





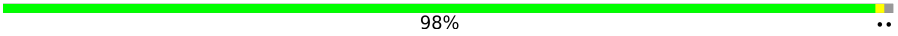
• Molecule 13: 50S ribosomal protein L4

Chain e:



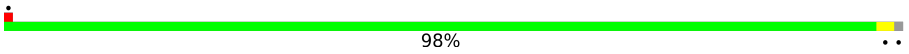
• Molecule 14: 50S ribosomal protein L5

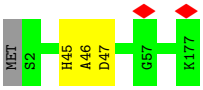
Chain f:



• Molecule 15: 50S ribosomal protein L6

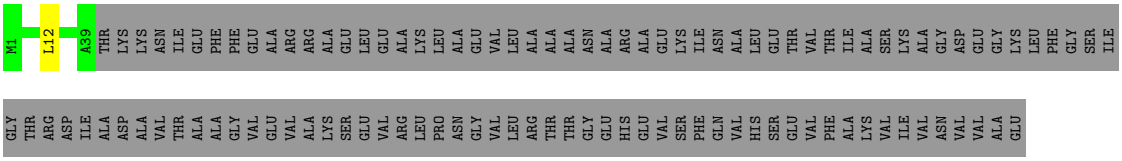
Chain g:





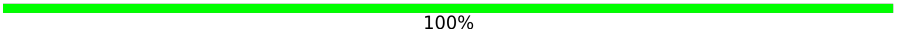
• Molecule 16: 50S ribosomal protein L9

Chain h:



• Molecule 17: 50S ribosomal protein L13

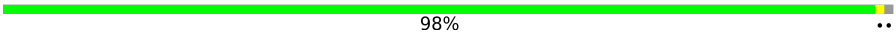
Chain j:

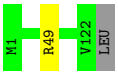


There are no outlier residues recorded for this chain.

• Molecule 18: 50S ribosomal protein L14

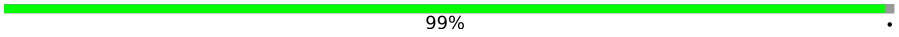
Chain k:





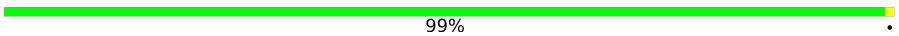
• Molecule 19: 50S ribosomal protein L15

Chain l:



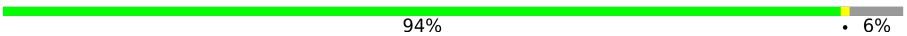
• Molecule 20: 50S ribosomal protein L16

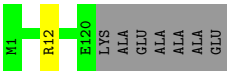
Chain m:



• Molecule 21: 50S ribosomal protein L17

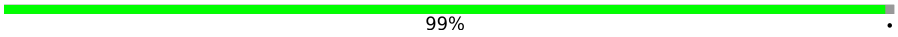
Chain n:





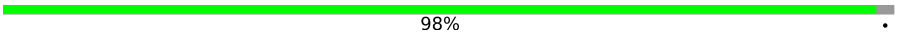
• Molecule 22: 50S ribosomal protein L18

Chain o:



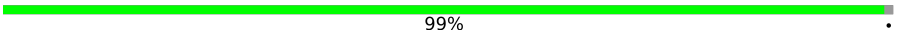
• Molecule 23: 50S ribosomal protein L19

Chain p:



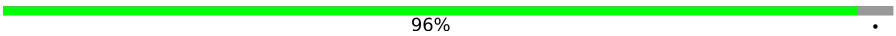
• Molecule 24: 50S ribosomal protein L20

Chain q:



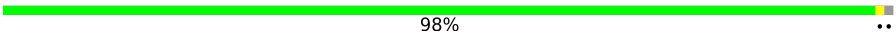
• Molecule 25: 50S ribosomal protein L21

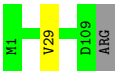
Chain r:



• Molecule 26: 50S ribosomal protein L22

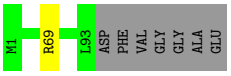
Chain s:





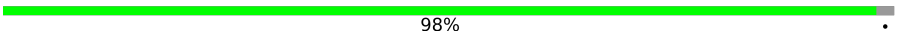
• Molecule 27: 50S ribosomal protein L23

Chain t:



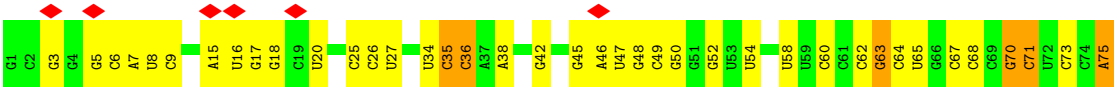
• Molecule 28: 50S ribosomal protein L24

Chain u:



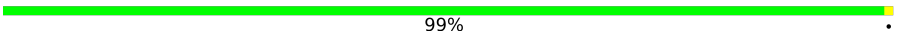
• Molecule 29: glycine-tRNA glyT

Chain v:



• Molecule 30: 50S ribosomal protein L25

Chain w:

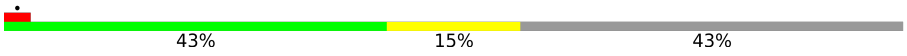


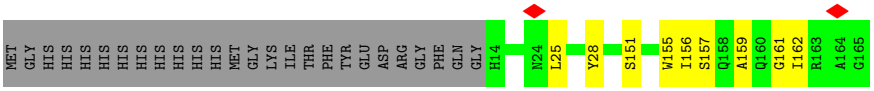
• Molecule 31: 50S ribosomal protein L27

Chain y:

• Molecule 32: Gamma-crystallin B

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	196254	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.034	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00741	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0	0.57	0/635	0.58	0/848
2	1	0.45	0/496	0.55	0/660
3	2	0.53	0/443	0.62	0/593
4	3	0.69	0/440	0.62	0/588
5	4	0.47	0/416	0.62	0/554
6	6	0.69	0/380	0.56	0/498
7	7	0.61	0/513	0.57	0/676
8	8	0.67	0/303	0.68	0/397
9	a	0.97	0/2824	1.07	3/4402 (0.1%)
10	b	1.42	1/69446 (0.0%)	1.22	537/108330 (0.5%)
11	c	0.66	0/2121	0.64	0/2852
12	d	0.65	0/1586	0.62	0/2134
13	e	0.59	0/1571	0.68	1/2113 (0.0%)
14	f	0.40	0/1434	0.63	0/1926
15	g	0.43	0/1343	0.74	2/1816 (0.1%)
16	h	0.44	0/290	0.74	0/392
17	j	0.63	0/1152	0.58	0/1551
18	k	0.62	0/947	0.64	0/1268
19	l	0.61	0/1051	0.65	0/1400
20	m	0.63	0/1093	0.58	0/1460
21	n	0.63	0/973	0.65	0/1301
22	o	0.44	0/902	0.62	0/1209
23	p	0.58	0/920	0.57	0/1231
24	q	0.76	0/960	0.63	0/1278
25	r	0.64	0/803	0.61	0/1070
26	s	0.60	0/852	0.58	0/1142
27	t	0.54	0/744	0.60	0/994
28	u	0.50	0/787	0.65	0/1051
29	v	0.64	0/1764	1.29	17/2744 (0.6%)
30	w	0.50	0/766	0.61	1/1025 (0.1%)
31	y	0.63	0/566	0.61	0/750
32	z	0.35	0/284	1.39	9/386 (2.3%)
All	All	1.24	1/98805 (0.0%)	1.11	570/148639 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	1	G	OP3-P	-10.15	1.49	1.61

All (570) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	g	45	HIS	N-CA-C	-12.39	77.55	111.00
32	z	159	ALA	N-CA-C	-11.50	79.94	111.00
10	b	2888	U	N3-C2-O2	-10.24	115.03	122.20
10	b	2027	C	N1-C2-O2	10.23	125.04	118.90
10	b	819	C	C6-N1-C2	-10.12	116.25	120.30
10	b	1315	U	N1-C2-O2	9.98	129.78	122.80
10	b	2462	G	O4'-C1'-N9	9.88	116.11	108.20
10	b	878	C	N1-C2-O2	9.76	124.76	118.90
10	b	849	U	N3-C2-O2	-9.70	115.41	122.20
10	b	2462	G	N7-C8-N9	9.68	117.94	113.10
10	b	1315	U	C2-N1-C1'	9.64	129.26	117.70
10	b	976	G	N7-C8-N9	9.63	117.91	113.10
32	z	156	ILE	N-CA-C	9.61	136.93	111.00
10	b	1315	U	N3-C2-O2	-9.52	115.53	122.20
10	b	2059	C	C6-N1-C2	-9.41	116.54	120.30
10	b	265	A	O4'-C1'-N9	9.39	115.71	108.20
10	b	2577	C	N1-C2-O2	9.31	124.49	118.90
10	b	2462	G	C8-N9-C4	-9.25	102.70	106.40
10	b	2577	C	C2-N1-C1'	9.08	128.78	118.80
32	z	28	TYR	N-CA-C	-8.98	86.76	111.00
10	b	2650	C	C6-N1-C2	-8.96	116.72	120.30
10	b	960	U	N1-C2-O2	8.91	129.03	122.80
10	b	2164	C	C5-C6-N1	8.87	125.44	121.00
29	v	36	C	N1-C2-O2	8.76	124.16	118.90
10	b	1781	U	C5-C6-N1	-8.75	118.33	122.70
10	b	2358	C	N1-C2-O2	8.59	124.06	118.90
10	b	849	U	N1-C2-O2	8.58	128.81	122.80
10	b	1818	C	N1-C2-O2	8.58	124.05	118.90
10	b	2164	C	C6-N1-C2	-8.52	116.89	120.30
10	b	2462	G	C5-N7-C8	-8.45	100.08	104.30
10	b	1776	C	C6-N1-C2	-8.39	116.94	120.30
10	b	1514	C	N1-C2-O2	8.36	123.92	118.90
10	b	2159	U	N1-C2-O2	8.32	128.63	122.80
10	b	976	G	C5-N7-C8	-8.30	100.15	104.30
10	b	878	C	C2-N1-C1'	8.30	127.92	118.80
10	b	2069	C	C6-N1-C2	-8.26	117.00	120.30
29	v	73	C	N1-C2-O2	8.24	123.84	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	g	46	ALA	N-CA-C	-8.23	88.78	111.00
10	b	976	G	C8-N9-C4	-8.13	103.15	106.40
29	v	58	U	N1-C2-O2	8.12	128.48	122.80
10	b	1641	C	N1-C2-O2	8.01	123.70	118.90
10	b	2650	C	C5-C6-N1	8.01	125.00	121.00
10	b	960	U	N3-C2-O2	-7.93	116.65	122.20
10	b	2510	U	N3-C2-O2	-7.92	116.65	122.20
10	b	830	U	N3-C2-O2	-7.89	116.68	122.20
10	b	830	U	C2-N1-C1'	7.89	127.17	117.70
10	b	830	U	N1-C2-O2	7.81	128.27	122.80
10	b	2358	C	N3-C2-O2	-7.79	116.44	121.90
10	b	1947	U	N3-C2-O2	-7.78	116.76	122.20
10	b	1587	C	N1-C2-O2	7.62	123.47	118.90
10	b	2159	U	N3-C2-O2	-7.60	116.88	122.20
10	b	201	C	C6-N1-C2	-7.59	117.26	120.30
10	b	2837	U	N1-C2-O2	7.59	128.11	122.80
10	b	1960	U	N3-C2-O2	-7.59	116.89	122.20
10	b	2027	C	N3-C2-O2	-7.57	116.60	121.90
10	b	2837	U	N3-C2-O2	-7.57	116.90	122.20
10	b	1456	C	N1-C2-O2	7.55	123.43	118.90
10	b	2290	G	C4-C5-N7	7.52	113.81	110.80
10	b	1456	C	O4'-C1'-N1	7.52	114.22	108.20
10	b	2510	U	N1-C2-O2	7.52	128.06	122.80
10	b	2379	G	C4-N9-C1'	7.52	136.27	126.50
10	b	2254	G	N3-C4-C5	7.50	132.35	128.60
10	b	1456	C	N3-C2-O2	-7.49	116.65	121.90
10	b	976	G	C4-C5-N7	7.49	113.80	110.80
10	b	2446	C	C6-N1-C2	-7.44	117.32	120.30
10	b	2379	G	N3-C4-C5	-7.44	124.88	128.60
10	b	1008	C	C6-N1-C2	-7.42	117.33	120.30
10	b	2577	C	N3-C2-O2	-7.42	116.71	121.90
32	z	155	TRP	N-CA-C	-7.42	90.98	111.00
10	b	874	U	C5-C6-N1	7.41	126.41	122.70
10	b	750	G	O4'-C1'-N9	7.41	114.12	108.20
10	b	390	U	N3-C2-O2	-7.39	117.03	122.20
29	v	35	C	N3-C2-O2	-7.39	116.73	121.90
10	b	912	A	O4'-C1'-N9	7.38	114.10	108.20
10	b	1641	C	N3-C2-O2	-7.35	116.75	121.90
10	b	984	C	N3-C2-O2	-7.31	116.78	121.90
10	b	625	C	C6-N1-C2	-7.29	117.38	120.30
10	b	2338	U	C2-N1-C1'	7.27	126.43	117.70
10	b	2837	U	C2-N1-C1'	7.26	126.41	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	v	36	C	N3-C2-O2	-7.26	116.82	121.90
10	b	2608	U	N3-C2-O2	-7.25	117.12	122.20
10	b	1316	C	C6-N1-C2	-7.25	117.40	120.30
10	b	1209	C	N1-C2-O2	7.23	123.24	118.90
10	b	346	A	N7-C8-N9	7.22	117.41	113.80
10	b	2254	G	C2-N3-C4	-7.19	108.31	111.90
10	b	2379	G	N3-C4-N9	7.15	130.29	126.00
10	b	1106	C	C6-N1-C2	-7.14	117.44	120.30
10	b	264	C	N1-C2-O2	7.14	123.18	118.90
10	b	1291	C	N1-C2-O2	7.14	123.18	118.90
29	v	35	C	N1-C2-O2	7.13	123.18	118.90
10	b	1316	C	C5-C6-N1	7.11	124.56	121.00
10	b	47	C	C6-N1-C2	-7.11	117.46	120.30
10	b	2888	U	N1-C2-O2	7.10	127.77	122.80
10	b	481	G	O4'-C1'-N9	7.10	113.88	108.20
10	b	917	C	N1-C2-O2	7.08	123.15	118.90
10	b	2608	U	N1-C2-O2	7.07	127.75	122.80
10	b	890	C	C6-N1-C2	-7.07	117.47	120.30
10	b	268	C	N1-C2-O2	7.06	123.14	118.90
10	b	1202	C	C6-N1-C2	-7.03	117.49	120.30
10	b	1094	C	C5-C6-N1	7.02	124.51	121.00
10	b	1646	C	N1-C2-O2	7.02	123.11	118.90
10	b	2059	C	C5-C6-N1	7.01	124.50	121.00
10	b	1461	G	N3-C4-C5	6.98	132.09	128.60
10	b	1119	C	C6-N1-C2	-6.98	117.51	120.30
10	b	1892	G	O4'-C1'-N9	6.98	113.78	108.20
10	b	2040	C	N1-C2-O2	6.97	123.08	118.90
10	b	343	C	N1-C2-O2	6.97	123.08	118.90
10	b	2871	G	C4-C5-N7	6.94	113.58	110.80
10	b	878	C	N3-C2-O2	-6.93	117.05	121.90
10	b	99	U	C2-N1-C1'	6.92	126.00	117.70
10	b	102	U	N1-C2-O2	6.92	127.64	122.80
13	e	124	PHE	N-CA-C	-6.92	92.33	111.00
10	b	1269	U	N3-C2-O2	-6.91	117.36	122.20
10	b	1730	C	C5-C6-N1	6.91	124.45	121.00
10	b	2563	C	N1-C2-O2	6.88	123.03	118.90
10	b	1514	C	N3-C2-O2	-6.85	117.11	121.90
10	b	1007	C	N1-C2-O2	6.81	122.99	118.90
10	b	373	U	N3-C2-O2	-6.81	117.43	122.20
10	b	239	C	N1-C2-O2	6.80	122.98	118.90
29	v	58	U	C2-N1-C1'	6.80	125.86	117.70
10	b	268	C	N3-C2-O2	-6.79	117.15	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	2610	C	C6-N1-C2	-6.78	117.59	120.30
10	b	417	C	O4'-C1'-N1	6.75	113.60	108.20
10	b	1646	C	N3-C2-O2	-6.73	117.19	121.90
29	v	58	U	N3-C2-O2	-6.73	117.49	122.20
10	b	1315	U	C6-N1-C1'	-6.71	111.80	121.20
10	b	559	C	C6-N1-C2	-6.70	117.62	120.30
10	b	209	C	C6-N1-C2	-6.70	117.62	120.30
10	b	2340	A	C5-N7-C8	-6.69	100.56	103.90
10	b	2640	C	N1-C2-O2	6.69	122.91	118.90
10	b	2583	C	C6-N1-C2	-6.67	117.63	120.30
10	b	1316	C	N1-C2-O2	6.67	122.90	118.90
10	b	2871	G	C4-N9-C1'	6.66	135.16	126.50
10	b	253	C	N1-C2-O2	6.66	122.89	118.90
10	b	2703	C	C6-N1-C2	-6.65	117.64	120.30
29	v	73	C	N3-C2-O2	-6.62	117.27	121.90
10	b	976	G	C4-N9-C1'	6.62	135.10	126.50
10	b	2727	C	C6-N1-C2	-6.61	117.66	120.30
29	v	73	C	C2-N1-C1'	6.61	126.07	118.80
10	b	1321	C	C6-N1-C2	-6.59	117.66	120.30
10	b	767	C	N1-C2-O2	6.58	122.85	118.90
10	b	264	C	N3-C2-O2	-6.58	117.29	121.90
10	b	562	C	C6-N1-C2	-6.58	117.67	120.30
10	b	2254	G	C4-C5-N7	6.58	113.43	110.80
10	b	2325	U	C2-N1-C1'	6.57	125.58	117.70
10	b	625	C	C5-C6-N1	6.56	124.28	121.00
10	b	637	C	C6-N1-C2	-6.56	117.68	120.30
10	b	1316	C	C2-N1-C1'	6.54	126.00	118.80
10	b	2510	U	C2-N1-C1'	6.51	125.52	117.70
10	b	2069	C	C5-C6-N1	6.50	124.25	121.00
10	b	2290	G	C5-N7-C8	-6.47	101.06	104.30
10	b	1384	G	O4'-C1'-N9	6.47	113.38	108.20
10	b	1577	C	N1-C2-O2	6.46	122.78	118.90
10	b	1732	C	N1-C2-O2	6.46	122.77	118.90
10	b	1456	C	C2-N1-C1'	6.45	125.90	118.80
10	b	1934	G	P-O3'-C3'	6.43	127.42	119.70
10	b	1301	G	C2'-C3'-O3'	6.43	123.99	113.70
10	b	2408	U	N1-C2-O2	6.43	127.30	122.80
10	b	559	C	C5-C6-N1	6.43	124.21	121.00
10	b	604	A	N7-C8-N9	6.43	117.01	113.80
10	b	2507	A	C2-N3-C4	6.41	113.81	110.60
10	b	2577	C	C6-N1-C1'	-6.41	113.11	120.80
10	b	2801	U	C5-C6-N1	6.41	125.90	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	2610	C	C5-C6-N1	6.41	124.20	121.00
10	b	1014	U	N3-C4-O4	-6.41	114.92	119.40
10	b	2150	C	C6-N1-C2	-6.38	117.75	120.30
10	b	1106	C	N1-C2-O2	6.38	122.73	118.90
10	b	102	U	N3-C2-O2	-6.38	117.74	122.20
10	b	891	C	N1-C2-O2	6.38	122.72	118.90
10	b	2743	U	N1-C2-O2	6.38	127.26	122.80
10	b	341	C	C6-N1-C2	-6.37	117.75	120.30
10	b	2871	G	C6-C5-N7	-6.36	126.58	130.40
10	b	22	C	C6-N1-C2	-6.36	117.76	120.30
10	b	1365	C	C6-N1-C2	-6.35	117.76	120.30
10	b	2379	G	C2-N3-C4	6.35	115.08	111.90
10	b	346	A	C8-N9-C4	-6.34	103.26	105.80
10	b	1978	C	N1-C2-O2	6.33	122.70	118.90
10	b	2254	G	C5-N7-C8	-6.32	101.14	104.30
10	b	323	C	C2-N1-C1'	6.32	125.75	118.80
10	b	2182	C	C2-N1-C1'	6.32	125.75	118.80
10	b	69	C	N1-C2-O2	6.31	122.68	118.90
10	b	2040	C	N3-C2-O2	-6.30	117.49	121.90
10	b	767	C	N3-C2-O2	-6.30	117.49	121.90
10	b	830	U	C6-N1-C1'	-6.30	112.38	121.20
10	b	343	C	C6-N1-C2	-6.29	117.78	120.30
10	b	586	C	C6-N1-C2	-6.28	117.79	120.30
10	b	343	C	N3-C2-O2	-6.28	117.50	121.90
10	b	1001	U	N3-C2-O2	-6.28	117.81	122.20
10	b	2340	A	N7-C8-N9	6.28	116.94	113.80
10	b	198	C	C5-C6-N1	6.27	124.14	121.00
10	b	849	U	C2-N1-C1'	6.25	125.20	117.70
10	b	1935	U	N1-C2-O2	6.25	127.17	122.80
10	b	341	C	C5-C6-N1	6.24	124.12	121.00
10	b	706	G	O4'-C1'-N9	6.24	113.19	108.20
10	b	1321	C	N1-C2-O2	6.24	122.64	118.90
10	b	921	U	N1-C2-O2	6.23	127.16	122.80
10	b	2358	C	C6-N1-C2	-6.23	117.81	120.30
10	b	1453	C	C2-N1-C1'	6.22	125.65	118.80
10	b	1609	C	C2-N1-C1'	6.22	125.64	118.80
10	b	2379	G	C8-N9-C1'	-6.22	118.92	127.00
10	b	2159	U	C2-N1-C1'	6.21	125.16	117.70
10	b	1347	C	C6-N1-C2	-6.20	117.82	120.30
10	b	2824	A	OP1-P-O3'	6.20	118.84	105.20
10	b	2047	C	C5-C6-N1	6.19	124.10	121.00
10	b	878	C	C6-N1-C1'	-6.19	113.38	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	739	C	C6-N1-C2	-6.18	117.83	120.30
10	b	1829	U	N1-C2-O2	6.18	127.13	122.80
10	b	2736	G	O4'-C1'-N9	6.18	113.14	108.20
10	b	1818	C	N3-C2-O2	-6.18	117.57	121.90
10	b	2736	G	C4-C5-N7	6.18	113.27	110.80
10	b	2874	C	C6-N1-C2	-6.17	117.83	120.30
10	b	1776	C	C5-C6-N1	6.17	124.08	121.00
10	b	99	U	N3-C2-O2	-6.16	117.89	122.20
32	z	151	SER	CB-CA-C	-6.14	98.43	110.10
10	b	2888	U	C2-N1-C1'	6.14	125.07	117.70
10	b	1462	U	N3-C2-O2	-6.13	117.91	122.20
10	b	2519	C	C6-N1-C2	-6.13	117.85	120.30
10	b	542	C	N1-C2-O2	6.11	122.56	118.90
10	b	1094	C	C6-N1-C2	-6.08	117.87	120.30
10	b	2577	C	C5-C6-N1	6.07	124.03	121.00
10	b	390	U	P-O3'-C3'	6.06	126.98	119.70
10	b	1701	G	C4-C5-N7	6.06	113.22	110.80
10	b	1321	C	C2-N1-C1'	6.05	125.46	118.80
10	b	1365	C	C5-C6-N1	6.05	124.03	121.00
10	b	1732	C	C2-N1-C1'	6.03	125.44	118.80
10	b	159	G	P-O3'-C3'	6.03	126.93	119.70
10	b	1797	C	C6-N1-C2	-6.03	117.89	120.30
29	v	36	C	C2-N1-C1'	6.02	125.43	118.80
10	b	742	C	N1-C2-O2	6.02	122.51	118.90
10	b	976	G	C6-C5-N7	-6.02	126.79	130.40
10	b	2640	C	C2-N1-C1'	6.02	125.42	118.80
10	b	510	C	N1-C2-O2	6.00	122.50	118.90
10	b	2381	A	O5'-P-OP2	-6.00	100.30	105.70
10	b	1898	C	N1-C2-O2	5.98	122.49	118.90
10	b	2151	A	C2-N3-C4	5.97	113.58	110.60
10	b	890	C	C5-C6-N1	5.96	123.98	121.00
10	b	1646	C	C6-N1-C2	-5.96	117.92	120.30
10	b	1960	U	N1-C2-O2	5.96	126.97	122.80
10	b	174	U	N3-C2-O2	-5.96	118.03	122.20
10	b	984	C	C2-N1-C1'	5.96	125.35	118.80
10	b	1832	C	C6-N1-C2	-5.95	117.92	120.30
10	b	1007	C	C6-N1-C2	-5.94	117.92	120.30
10	b	917	C	N3-C2-O2	-5.94	117.74	121.90
10	b	1453	C	C4-C5-C6	5.94	120.37	117.40
32	z	151	SER	N-CA-C	5.94	127.03	111.00
10	b	490	C	N1-C2-O2	5.94	122.46	118.90
10	b	1296	U	N3-C2-O2	-5.93	118.05	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	1155	C	C6-N1-C2	-5.93	117.93	120.30
10	b	2766	C	C6-N1-C2	-5.93	117.93	120.30
10	b	1001	U	N1-C2-O2	5.92	126.94	122.80
10	b	2048	C	C6-N1-C2	-5.92	117.93	120.30
10	b	705	U	P-O3'-C3'	5.91	126.79	119.70
10	b	2630	C	C6-N1-C2	-5.90	117.94	120.30
10	b	917	C	C2-N1-C1'	5.90	125.29	118.80
10	b	1870	C	N1-C2-O2	5.89	122.44	118.90
10	b	1400	C	N1-C2-O2	5.89	122.44	118.90
10	b	1106	C	C5-C6-N1	5.89	123.94	121.00
10	b	1730	C	C6-N1-C2	-5.89	117.94	120.30
10	b	268	C	C6-N1-C2	-5.89	117.94	120.30
10	b	1706	C	P-O3'-C3'	5.89	126.76	119.70
10	b	1912	C	N1-C2-O2	5.88	122.43	118.90
10	b	604	A	C5-N7-C8	-5.88	100.96	103.90
10	b	967	C	N1-C2-O2	5.88	122.42	118.90
10	b	2502	C	N1-C2-O2	5.87	122.42	118.90
10	b	2743	U	N3-C2-O2	-5.87	118.09	122.20
10	b	2516	C	C6-N1-C2	-5.87	117.95	120.30
10	b	1008	C	C5-C6-N1	5.86	123.93	121.00
9	a	66	A	P-O3'-C3'	5.86	126.73	119.70
10	b	681	C	N1-C2-O2	5.86	122.42	118.90
10	b	948	C	C6-N1-C2	-5.84	117.96	120.30
10	b	816	C	N1-C2-O2	5.84	122.40	118.90
10	b	1781	U	C4-C5-C6	5.84	123.20	119.70
10	b	228	C	P-O3'-C3'	5.83	126.70	119.70
10	b	681	C	N3-C2-O2	-5.83	117.82	121.90
10	b	554	U	N3-C2-O2	-5.82	118.12	122.20
10	b	1384	G	C4-C5-N7	5.82	113.13	110.80
10	b	209	C	C5-C6-N1	5.82	123.91	121.00
10	b	346	A	C5-N7-C8	-5.81	101.00	103.90
10	b	1892	G	N7-C8-N9	5.80	116.00	113.10
10	b	413	C	C6-N1-C2	-5.80	117.98	120.30
10	b	1677	C	N3-C2-O2	-5.79	117.84	121.90
10	b	542	C	N3-C2-O2	-5.79	117.85	121.90
10	b	1883	C	C6-N1-C2	-5.79	117.98	120.30
10	b	2010	C	N3-C2-O2	-5.79	117.85	121.90
10	b	1321	C	N3-C2-O2	-5.79	117.85	121.90
10	b	2736	G	C5-N7-C8	-5.78	101.41	104.30
10	b	917	C	C6-N1-C2	-5.77	117.99	120.30
10	b	2408	U	N3-C2-O2	-5.77	118.16	122.20
10	b	1453	C	N3-C2-O2	-5.77	117.86	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	1236	U	N1-C2-O2	5.76	126.84	122.80
10	b	1014	U	C5-C4-O4	5.75	129.35	125.90
10	b	1646	C	C2-N1-C1'	5.75	125.13	118.80
10	b	2619	U	C5-C6-N1	5.75	125.58	122.70
10	b	1788	A	O4'-C1'-N9	5.75	112.80	108.20
10	b	2871	G	N7-C8-N9	5.75	115.97	113.10
10	b	2004	C	N1-C2-O2	5.75	122.35	118.90
10	b	960	U	C5-C6-N1	5.74	125.57	122.70
10	b	1829	U	N3-C2-O2	-5.74	118.18	122.20
10	b	2563	C	N3-C2-O2	-5.74	117.88	121.90
10	b	2566	U	N3-C2-O2	-5.74	118.18	122.20
10	b	1269	U	N1-C2-O2	5.74	126.82	122.80
29	v	71	C	N1-C2-O2	5.73	122.34	118.90
29	v	75	A	OP1-P-OP2	-5.73	111.00	119.60
10	b	2507	A	N1-C2-N3	-5.73	126.44	129.30
10	b	1007	C	N3-C2-O2	-5.72	117.89	121.90
10	b	2001	C	N1-C2-O2	5.72	122.33	118.90
10	b	1154	C	C6-N1-C2	-5.71	118.02	120.30
10	b	967	C	N3-C2-O2	-5.71	117.91	121.90
29	v	63	G	C4-N9-C1'	5.70	133.91	126.50
10	b	786	G	C5-N7-C8	-5.69	101.45	104.30
10	b	837	C	N1-C2-O2	5.69	122.32	118.90
10	b	1236	U	N3-C2-O2	-5.69	118.22	122.20
9	a	117	G	C8-N9-C1'	5.68	134.39	127.00
10	b	1996	G	O4'-C1'-N9	-5.68	103.66	108.20
10	b	1236	U	C2-N1-C1'	5.68	124.52	117.70
10	b	2110	U	P-O3'-C3'	5.67	126.51	119.70
10	b	2460	C	N3-C2-O2	-5.67	117.93	121.90
10	b	413	C	C5-C6-N1	5.67	123.84	121.00
10	b	373	U	O5'-P-OP2	-5.67	100.60	105.70
10	b	2328	U	OP2-P-O3'	5.67	117.67	105.20
10	b	1454	G	C4-C5-N7	5.66	113.07	110.80
10	b	1978	C	N3-C2-O2	-5.66	117.94	121.90
10	b	1461	G	C6-N1-C2	5.66	128.50	125.10
10	b	69	C	N3-C2-O2	-5.66	117.94	121.90
10	b	2046	A	N1-C6-N6	5.66	121.99	118.60
10	b	913	A	N7-C8-N9	5.65	116.63	113.80
10	b	1119	C	N1-C2-O2	5.65	122.29	118.90
10	b	1892	G	C4-N9-C1'	5.65	133.84	126.50
10	b	1587	C	C5-C6-N1	5.64	123.82	121.00
10	b	2340	A	C4-C5-N7	5.64	113.52	110.70
10	b	2720	C	N1-C2-O2	5.64	122.28	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	2801	U	C2-N1-C1'	5.62	124.45	117.70
10	b	99	U	N1-C2-O2	5.62	126.73	122.80
10	b	921	U	N3-C2-O2	-5.61	118.27	122.20
10	b	953	C	N1-C2-O2	5.60	122.26	118.90
10	b	1514	C	C2-N1-C1'	5.60	124.96	118.80
10	b	164	C	N1-C2-O2	5.60	122.26	118.90
10	b	1577	C	N3-C2-O2	-5.59	117.98	121.90
10	b	1354	U	N3-C2-O2	-5.58	118.29	122.20
10	b	786	G	C4-C5-N7	5.58	113.03	110.80
10	b	205	G	O4'-C1'-N9	5.58	112.66	108.20
10	b	510	C	N3-C2-O2	-5.57	118.00	121.90
10	b	1759	A	O4'-C1'-N9	5.57	112.65	108.20
10	b	1384	G	C5-N7-C8	-5.56	101.52	104.30
9	a	15	A	O4'-C1'-N9	5.56	112.65	108.20
10	b	1587	C	N3-C2-O2	-5.56	118.01	121.90
10	b	1209	C	N3-C2-O2	-5.56	118.01	121.90
32	z	161	GLY	N-CA-C	5.56	126.99	113.10
10	b	2109	U	N1-C2-O2	5.55	126.68	122.80
29	v	73	C	C6-N1-C2	-5.54	118.08	120.30
10	b	1461	G	N3-C4-N9	-5.54	122.68	126.00
10	b	1293	C	C6-N1-C2	-5.53	118.09	120.30
10	b	2577	C	C6-N1-C2	-5.53	118.09	120.30
10	b	2884	C	N1-C2-O2	5.53	122.22	118.90
10	b	1345	G	C4-N9-C1'	5.53	133.69	126.50
10	b	253	C	N3-C2-O2	-5.52	118.04	121.90
10	b	114	U	C2-N1-C1'	5.51	124.31	117.70
10	b	542	C	C6-N1-C2	-5.51	118.10	120.30
10	b	1308	C	N1-C2-O2	5.51	122.20	118.90
10	b	984	C	C6-N1-C2	-5.50	118.10	120.30
10	b	2445	U	N1-C2-O2	5.50	126.65	122.80
10	b	2460	C	N1-C2-O2	5.50	122.20	118.90
10	b	2771	C	N1-C2-O2	5.50	122.20	118.90
10	b	2012	C	C6-N1-C2	-5.50	118.10	120.30
10	b	2047	C	C6-N1-C2	-5.49	118.10	120.30
10	b	2338	U	N1-C2-O2	5.49	126.64	122.80
10	b	1455	A	N7-C8-N9	5.49	116.55	113.80
32	z	162	ILE	N-CA-C	5.49	125.82	111.00
10	b	2642	G	O4'-C1'-N9	5.48	112.59	108.20
10	b	2778	C	C6-N1-C2	-5.48	118.11	120.30
10	b	1499	U	N3-C2-O2	-5.48	118.36	122.20
10	b	1771	U	N1-C2-O2	5.48	126.63	122.80
10	b	66	C	N1-C2-O2	5.46	122.17	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	v	63	G	C8-N9-C1'	-5.46	119.91	127.00
10	b	198	C	C6-N1-C2	-5.45	118.12	120.30
10	b	1354	U	N1-C2-O2	5.45	126.62	122.80
10	b	2185	U	P-O3'-C3'	5.45	126.25	119.70
10	b	1944	U	N3-C2-O2	-5.45	118.38	122.20
32	z	159	ALA	CB-CA-C	5.45	118.28	110.10
10	b	636	C	C6-N1-C2	-5.45	118.12	120.30
10	b	2399	C	C6-N1-C2	-5.45	118.12	120.30
10	b	1935	U	N3-C2-O2	-5.45	118.39	122.20
10	b	2420	C	C5-C6-N1	5.44	123.72	121.00
10	b	1781	U	C2-N3-C4	-5.44	123.74	127.00
10	b	612	C	C5-C6-N1	5.44	123.72	121.00
10	b	1064	G	N3-C4-N9	5.44	129.26	126.00
10	b	674	C	C6-N1-C2	-5.43	118.13	120.30
10	b	1672	C	N1-C2-O2	5.43	122.16	118.90
10	b	1381	U	N1-C2-O2	5.42	126.60	122.80
10	b	1587	C	C2-N1-C1'	5.42	124.77	118.80
10	b	953	C	N3-C2-O2	-5.42	118.11	121.90
10	b	1701	G	C5-N7-C8	-5.42	101.59	104.30
10	b	2338	U	C6-N1-C1'	-5.41	113.62	121.20
10	b	2868	G	P-O3'-C3'	5.41	126.20	119.70
10	b	2871	G	C5-N7-C8	-5.41	101.59	104.30
10	b	1102	C	C5-C6-N1	5.41	123.70	121.00
10	b	2871	G	C8-N9-C1'	-5.41	119.97	127.00
10	b	1308	C	N3-C2-O2	-5.41	118.12	121.90
10	b	268	C	C2-N1-C1'	5.40	124.74	118.80
10	b	486	C	N1-C2-O2	5.40	122.14	118.90
10	b	1566	C	C5-C6-N1	5.40	123.70	121.00
10	b	166	U	C5-C6-N1	5.40	125.40	122.70
10	b	1007	C	C5-C6-N1	5.40	123.70	121.00
10	b	1609	C	N1-C2-O2	5.40	122.14	118.90
10	b	2511	C	N1-C2-O2	5.39	122.14	118.90
10	b	1989	C	N1-C2-O2	5.39	122.14	118.90
10	b	1064	G	C4-N9-C1'	5.38	133.50	126.50
10	b	1202	C	C5-C6-N1	5.38	123.69	121.00
10	b	819	C	C5-C6-N1	5.38	123.69	121.00
10	b	1832	C	C5-C6-N1	5.38	123.69	121.00
10	b	1912	C	N3-C2-O2	-5.38	118.14	121.90
10	b	2290	G	C6-C5-N7	-5.38	127.17	130.40
10	b	2216	A	N7-C8-N9	5.37	116.48	113.80
10	b	2462	G	C4-N9-C1'	5.37	133.48	126.50
10	b	682	C	C6-N1-C2	-5.37	118.15	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	2328	U	P-O3'-C3'	5.37	126.14	119.70
10	b	1771	U	N3-C2-O2	-5.36	118.45	122.20
10	b	778	G	C6-C5-N7	-5.36	127.18	130.40
10	b	360	U	N1-C2-O2	5.36	126.55	122.80
10	b	814	C	C5-C6-N1	5.36	123.68	121.00
10	b	1998	C	N1-C2-O2	5.36	122.11	118.90
10	b	1000	C	C6-N1-C2	-5.35	118.16	120.30
10	b	114	U	C5-C6-N1	5.34	125.37	122.70
10	b	1320	U	C5-C6-N1	5.34	125.37	122.70
10	b	27	G	P-O3'-C3'	5.34	126.11	119.70
10	b	1381	U	N3-C2-O2	-5.34	118.47	122.20
10	b	510	C	C6-N1-C2	-5.32	118.17	120.30
10	b	2358	C	C2-N1-C1'	5.32	124.65	118.80
10	b	2003	C	C5-C6-N1	5.32	123.66	121.00
10	b	1602	C	C6-N1-C2	-5.32	118.17	120.30
10	b	2077	C	C6-N1-C2	-5.31	118.18	120.30
10	b	1320	U	N1-C2-O2	5.31	126.52	122.80
10	b	2539	G	P-O3'-C3'	5.30	126.06	119.70
10	b	2682	C	N1-C2-O2	5.30	122.08	118.90
10	b	2736	G	C5-C6-N1	5.29	114.15	111.50
10	b	213	A	C8-N9-C4	5.29	107.92	105.80
10	b	2107	C	C6-N1-C2	-5.29	118.19	120.30
10	b	1892	G	C6-C5-N7	-5.29	127.23	130.40
10	b	2244	U	N1-C2-O2	5.29	126.50	122.80
10	b	2595	C	C6-N1-C2	-5.29	118.19	120.30
10	b	2236	C	C6-N1-C2	-5.28	118.19	120.30
10	b	562	C	C5-C6-N1	5.27	123.64	121.00
10	b	2312	G	C8-N9-C4	-5.27	104.29	106.40
10	b	590	U	C2-N1-C1'	5.27	124.02	117.70
10	b	1528	C	C6-N1-C2	-5.27	118.19	120.30
10	b	1898	C	N3-C2-O2	-5.27	118.21	121.90
10	b	648	U	C6-N1-C2	-5.26	117.84	121.00
10	b	2446	C	C5-C6-N1	5.26	123.63	121.00
10	b	2109	U	N3-C2-O2	-5.26	118.52	122.20
10	b	1810	A	C5-C6-N6	-5.26	119.49	123.70
10	b	202	U	N3-C2-O2	-5.26	118.52	122.20
10	b	2338	U	N3-C2-O2	-5.25	118.52	122.20
10	b	1032	C	C6-N1-C2	-5.25	118.20	120.30
29	v	70	G	C4-N9-C1'	5.25	133.32	126.50
10	b	1119	C	N3-C2-O2	-5.25	118.23	121.90
10	b	1892	G	C5-N7-C8	-5.25	101.68	104.30
10	b	2265	C	N1-C2-O2	5.25	122.05	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	2462	G	C4-C5-N7	5.25	112.90	110.80
10	b	484	C	C5-C6-N1	5.24	123.62	121.00
10	b	1297	C	N1-C2-O2	5.24	122.05	118.90
10	b	174	U	N1-C2-O2	5.24	126.47	122.80
10	b	373	U	N1-C2-O2	5.24	126.47	122.80
30	w	66	ASP	CB-CG-OD2	5.24	123.01	118.30
10	b	2408	U	C2-N1-C1'	5.23	123.98	117.70
10	b	1597	C	P-O3'-C3'	5.23	125.97	119.70
10	b	1396	U	C5-C6-N1	5.22	125.31	122.70
10	b	61	C	N1-C2-O2	5.22	122.03	118.90
10	b	2433	G	OP2-P-O3'	5.22	116.68	105.20
10	b	1291	C	N3-C2-O2	-5.22	118.25	121.90
10	b	1928	C	C6-N1-C2	-5.21	118.21	120.30
10	b	2797	C	N1-C2-O2	5.21	122.03	118.90
10	b	2649	G	N3-C4-C5	5.21	131.21	128.60
10	b	786	G	N7-C8-N9	5.21	115.70	113.10
10	b	1280	C	N1-C2-O2	5.21	122.03	118.90
10	b	1345	G	C8-N9-C1'	-5.21	120.23	127.00
10	b	1166	C	C6-N1-C2	-5.21	118.22	120.30
10	b	1119	C	C5-C6-N1	5.20	123.60	121.00
10	b	1453	C	C6-N1-C1'	-5.20	114.56	120.80
10	b	2047	C	N1-C2-O2	5.20	122.02	118.90
10	b	2727	C	C5-C6-N1	5.20	123.60	121.00
10	b	1540	G	P-O3'-C3'	5.20	125.94	119.70
10	b	750	G	N1-C6-O6	-5.19	116.79	119.90
10	b	754	A	C5-N7-C8	-5.19	101.31	103.90
10	b	1416	C	C5-C6-N1	5.19	123.59	121.00
10	b	2619	U	C2-N1-C1'	5.18	123.92	117.70
10	b	1892	G	C8-N9-C4	-5.18	104.33	106.40
10	b	2224	U	N3-C2-O2	-5.18	118.57	122.20
10	b	2428	C	N1-C2-O2	5.18	122.01	118.90
10	b	2580	G	C4-N9-C1'	5.17	133.22	126.50
10	b	590	U	C5-C6-N1	5.17	125.28	122.70
10	b	645	A	O4'-C1'-N9	5.17	112.33	108.20
10	b	1297	C	N3-C2-O2	-5.17	118.28	121.90
10	b	2620	C	C6-N1-C2	-5.17	118.23	120.30
10	b	1587	C	C6-N1-C2	-5.17	118.23	120.30
10	b	583	C	N3-C2-O2	-5.16	118.28	121.90
10	b	1672	C	N3-C2-O2	-5.16	118.29	121.90
10	b	2254	G	C6-N1-C2	5.16	128.20	125.10
10	b	102	U	C5-C6-N1	5.16	125.28	122.70
10	b	276	U	C5-C6-N1	5.16	125.28	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	9	G	P-O3'-C3'	5.15	125.89	119.70
10	b	704	U	N1-C2-O2	5.15	126.41	122.80
10	b	1671	A	C8-N9-C4	-5.15	103.74	105.80
10	b	898	A	C4-N9-C1'	5.15	135.57	126.30
10	b	2801	U	N1-C2-O2	5.15	126.40	122.80
10	b	2254	G	N3-C4-N9	-5.14	122.91	126.00
10	b	2884	C	N3-C2-O2	-5.14	118.30	121.90
10	b	967	C	C6-N1-C2	-5.14	118.24	120.30
10	b	1558	C	N3-C2-O2	-5.14	118.30	121.90
10	b	1078	C	C6-N1-C2	-5.14	118.25	120.30
10	b	814	C	C6-N1-C2	-5.13	118.25	120.30
10	b	2484	C	N3-C2-O2	-5.13	118.31	121.90
10	b	2511	C	N3-C2-O2	-5.13	118.31	121.90
10	b	786	G	C8-N9-C4	-5.13	104.35	106.40
10	b	1929	C	C6-N1-C2	-5.12	118.25	120.30
10	b	2888	U	C5-C4-O4	5.12	128.97	125.90
10	b	2093	C	N3-C2-O2	-5.12	118.32	121.90
10	b	239	C	N3-C2-O2	-5.12	118.32	121.90
10	b	2518	U	C6-N1-C2	-5.12	117.93	121.00
10	b	1896	C	C5-C6-N1	5.12	123.56	121.00
10	b	481	G	C4-N9-C1'	-5.11	119.86	126.50
10	b	69	C	C6-N1-C2	-5.11	118.26	120.30
10	b	459	U	N3-C2-O2	-5.11	118.63	122.20
10	b	2510	U	C6-N1-C2	-5.10	117.94	121.00
10	b	1308	C	C6-N1-C2	-5.09	118.26	120.30
10	b	1455	A	C5-N7-C8	-5.09	101.36	103.90
10	b	378	C	C6-N1-C2	-5.09	118.26	120.30
10	b	2143	U	N1-C2-O2	5.09	126.36	122.80
10	b	1563	C	C5-C6-N1	5.09	123.54	121.00
10	b	2182	C	N1-C2-O2	5.09	121.95	118.90
10	b	1968	G	O4'-C1'-N9	-5.08	104.14	108.20
10	b	1280	C	N3-C2-O2	-5.07	118.35	121.90
10	b	597	C	C6-N1-C2	-5.06	118.27	120.30
10	b	2878	C	N1-C2-O2	5.06	121.94	118.90
10	b	418	C	C6-N1-C2	-5.06	118.28	120.30
10	b	2736	G	N7-C8-N9	5.06	115.63	113.10
10	b	1106	C	N3-C2-O2	-5.05	118.36	121.90
10	b	726	U	C2-N1-C1'	5.05	123.76	117.70
10	b	390	U	N1-C2-O2	5.05	126.33	122.80
10	b	1672	C	C6-N1-C2	-5.05	118.28	120.30
10	b	1998	C	N3-C2-O2	-5.04	118.37	121.90
10	b	2420	C	C6-N1-C2	-5.04	118.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	397	U	C5-C6-N1	5.04	125.22	122.70
10	b	1439	C	N1-C2-O2	5.04	121.93	118.90
10	b	2001	C	N3-C2-O2	-5.04	118.37	121.90
10	b	1242	U	C2-N1-C1'	5.04	123.75	117.70
10	b	604	A	C8-N9-C4	-5.04	103.78	105.80
10	b	2566	U	N1-C2-O2	5.04	126.33	122.80
10	b	391	A	N7-C8-N9	5.04	116.32	113.80
10	b	1074	C	N1-C2-O2	5.04	121.92	118.90
10	b	2421	C	C6-N1-C2	-5.04	118.29	120.30
10	b	323	C	C6-N1-C1'	-5.03	114.76	120.80
10	b	1764	A	P-O3'-C3'	5.03	125.74	119.70
10	b	976	G	O4'-C1'-N9	5.02	112.22	108.20
10	b	1321	C	C5-C6-N1	5.02	123.51	121.00
10	b	223	A	O4'-C1'-N9	5.02	112.22	108.20
10	b	1047	C	N3-C4-C5	5.02	123.91	121.90
10	b	1359	C	N1-C2-O2	5.02	121.91	118.90
10	b	705	U	C2'-C3'-O3'	5.02	121.73	113.70
10	b	1544	U	N1-C2-O2	5.02	126.31	122.80
10	b	225	C	N1-C2-O2	5.02	121.91	118.90
10	b	1613	C	N1-C2-O2	5.02	121.91	118.90
10	b	1381	U	C2-N1-C1'	5.02	123.72	117.70
10	b	939	C	C6-N1-C2	-5.01	118.29	120.30
10	b	1693	C	C6-N1-C2	-5.01	118.30	120.30
10	b	963	C	O5'-P-OP2	-5.01	101.19	105.70
10	b	1839	C	C6-N1-C2	-5.01	118.30	120.30
10	b	343	C	C5-C6-N1	5.01	123.50	121.00
10	b	1718	U	N1-C2-O2	5.01	126.31	122.80
10	b	1439	C	C2-N1-C1'	5.00	124.31	118.80
10	b	2308	G	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	625	0	652	2	0
2	1	495	0	526	6	0
3	2	439	0	482	1	0
4	3	434	0	445	4	0
5	4	409	0	440	2	0
6	6	377	0	418	2	0
7	7	504	0	572	5	0
8	8	302	0	341	1	0
9	a	2528	0	1283	0	0
10	b	62008	0	31185	0	0
11	c	2082	0	2154	0	0
12	d	1565	0	1616	0	0
13	e	1552	0	1619	0	0
14	f	1410	0	1444	0	0
15	g	1323	0	1371	0	0
16	h	287	0	307	0	0
17	j	1129	0	1162	0	0
18	k	938	0	1012	0	0
19	l	1042	0	1121	0	0
20	m	1074	0	1157	0	0
21	n	960	0	1000	0	0
22	o	892	0	923	0	0
23	p	908	0	956	0	0
24	q	947	0	1019	0	0
25	r	791	0	811	0	0
26	s	845	0	908	0	0
27	t	738	0	807	0	0
28	u	779	0	831	0	0
29	v	1583	0	807	0	0
30	w	753	0	780	0	0
31	y	559	0	575	0	0
32	z	275	0	247	0	0
All	All	90553	0	58971	23	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:12:SER:HB3	3:2:32:ILE:HD11	1.88	0.56
2:1:14:LEU:HD11	2:1:56:LEU:HD23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:9:LYS:HE3	2:1:13:GLU:HG2	1.90	0.52
6:6:1:MET:SD	6:6:1:MET:N	2.74	0.51
2:1:49:ASP:OD1	2:1:52:ARG:NH2	2.43	0.51
4:3:54:VAL:HG23	4:3:55:ILE:HG12	1.92	0.50
2:1:21:LEU:HB3	2:1:50:VAL:HG12	1.94	0.50
5:4:37:LYS:HG2	5:4:48:ILE:HG13	1.93	0.49
4:3:52:ARG:HH11	4:3:54:VAL:HA	1.80	0.46
7:7:32:ILE:HG22	7:7:32:ILE:O	2.16	0.46
6:6:25:LYS:HB3	6:6:25:LYS:HE3	1.82	0.45
4:3:38:HIS:ND1	4:3:39:LEU:O	2.37	0.45
2:1:14:LEU:HD21	2:1:56:LEU:HG	1.98	0.45
8:8:4:ARG:O	8:8:38:GLY:N	2.49	0.45
7:7:31:HIS:H	7:7:31:HIS:CD2	2.36	0.44
1:0:3:ARG:CD	1:0:30:LEU:HD23	2.48	0.44
4:3:37:LYS:HB2	4:3:37:LYS:HE3	1.84	0.42
7:7:30:ARG:HD2	7:7:30:ARG:HA	1.75	0.42
1:0:72:ARG:HG3	1:0:78:TYR:HE2	1.83	0.42
2:1:60:LYS:HB3	2:1:60:LYS:HE2	1.84	0.42
5:4:9:ILE:HA	5:4:53:LYS:HB2	2.02	0.41
7:7:31:HIS:H	7:7:31:HIS:HD2	1.69	0.41
7:7:8:ARG:HD2	7:7:8:ARG:HA	1.90	0.40

There are no symmetry-related clashes.

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	
1	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
2	1	59/63 (94%)	53 (90%)	6 (10%)	0	100	100
3	2	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
4	3	53/57 (93%)	51 (96%)	2 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	4	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
6	6	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
7	7	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
8	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	c	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
12	d	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
13	e	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
14	f	175/179 (98%)	155 (89%)	20 (11%)	0	100	100
15	g	174/177 (98%)	160 (92%)	13 (8%)	1 (1%)	25	45
16	h	37/149 (25%)	33 (89%)	4 (11%)	0	100	100
17	j	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	k	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
19	l	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
20	m	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
21	n	118/127 (93%)	104 (88%)	14 (12%)	0	100	100
22	o	114/117 (97%)	104 (91%)	10 (9%)	0	100	100
23	p	111/115 (96%)	106 (96%)	5 (4%)	0	100	100
24	q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
25	r	95/103 (92%)	85 (90%)	10 (10%)	0	100	100
26	s	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
27	t	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
28	u	100/104 (96%)	80 (80%)	20 (20%)	0	100	100
30	w	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
31	y	72/85 (85%)	67 (93%)	5 (7%)	0	100	100
32	z	33/61 (54%)	25 (76%)	8 (24%)	0	100	100
All	All	3076/3328 (92%)	2855 (93%)	220 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	g	47	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	67/68 (98%)	66 (98%)	1 (2%)	65 82
2	1	54/55 (98%)	54 (100%)	0	100 100
3	2	47/49 (96%)	47 (100%)	0	100 100
4	3	46/48 (96%)	45 (98%)	1 (2%)	52 74
5	4	45/49 (92%)	45 (100%)	0	100 100
6	6	38/38 (100%)	38 (100%)	0	100 100
7	7	51/52 (98%)	49 (96%)	2 (4%)	32 56
8	8	34/34 (100%)	34 (100%)	0	100 100
11	c	216/218 (99%)	216 (100%)	0	100 100
12	d	164/164 (100%)	162 (99%)	2 (1%)	71 86
13	e	165/165 (100%)	162 (98%)	3 (2%)	59 78
14	f	148/150 (99%)	146 (99%)	2 (1%)	67 84
15	g	137/138 (99%)	137 (100%)	0	100 100
16	h	30/114 (26%)	29 (97%)	1 (3%)	38 61
17	j	116/116 (100%)	116 (100%)	0	100 100
18	k	103/104 (99%)	102 (99%)	1 (1%)	76 89
19	l	102/103 (99%)	102 (100%)	0	100 100
20	m	109/109 (100%)	108 (99%)	1 (1%)	78 90
21	n	100/103 (97%)	99 (99%)	1 (1%)	76 89
22	o	86/87 (99%)	86 (100%)	0	100 100
23	p	98/100 (98%)	98 (100%)	0	100 100
24	q	89/90 (99%)	89 (100%)	0	100 100
25	r	82/84 (98%)	82 (100%)	0	100 100
26	s	92/93 (99%)	91 (99%)	1 (1%)	73 88
27	t	80/84 (95%)	79 (99%)	1 (1%)	69 85
28	u	83/85 (98%)	83 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	w	78/78 (100%)	78 (100%)	0	100 100
31	y	55/63 (87%)	54 (98%)	1 (2%)	59 78
32	z	31/53 (58%)	29 (94%)	2 (6%)	17 33
All	All	2546/2694 (94%)	2526 (99%)	20 (1%)	82 92

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	ARG
4	3	10	ARG
7	7	30	ARG
7	7	31	HIS
12	d	121	THR
12	d	184	ARG
13	e	134	LEU
13	e	137	LYS
13	e	138	LEU
14	f	115	ARG
14	f	169	LEU
16	h	12	LEU
18	k	49	ARG
20	m	75	GLU
21	n	12	ARG
26	s	29	VAL
27	t	69	ARG
31	y	51	VAL
32	z	25	LEU
32	z	157	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	26	ASN
14	f	27	GLN
14	f	135	GLN
15	g	73	ASN
32	z	24	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	2882/2906 (99%)	765 (26%)	0
29	v	74/75 (98%)	37 (50%)	0
9	a	116/120 (96%)	33 (28%)	0
All	All	3072/3101 (99%)	835 (27%)	0

All (835) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	a	4	C
9	a	5	U
9	a	7	G
9	a	9	G
9	a	13	G
9	a	24	G
9	a	25	U
9	a	26	C
9	a	29	A
9	a	30	C
9	a	35	C
9	a	39	A
9	a	42	C
9	a	43	C
9	a	44	G
9	a	52	A
9	a	53	A
9	a	56	G
9	a	66	A
9	a	67	G
9	a	87	U
9	a	88	C
9	a	89	U
9	a	90	C
9	a	91	C
9	a	93	C
9	a	99	A
9	a	109	A
9	a	112	G
9	a	113	C
9	a	114	C
9	a	117	G
9	a	118	C
10	b	4	U
10	b	10	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	12	U
10	b	15	G
10	b	28	A
10	b	34	U
10	b	35	G
10	b	46	G
10	b	51	G
10	b	62	U
10	b	63	A
10	b	71	A
10	b	74	A
10	b	75	G
10	b	84	A
10	b	91	A
10	b	92	U
10	b	93	G
10	b	100	U
10	b	101	A
10	b	102	U
10	b	103	A
10	b	118	A
10	b	119	A
10	b	120	U
10	b	121	G
10	b	122	G
10	b	125	A
10	b	136	G
10	b	137	U
10	b	142	A
10	b	144	A
10	b	159	G
10	b	160	A
10	b	163	C
10	b	174	U
10	b	175	G
10	b	177	G
10	b	196	A
10	b	199	A
10	b	215	G
10	b	216	A
10	b	221	A
10	b	222	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	223	A
10	b	224	U
10	b	229	C
10	b	230	G
10	b	233	A
10	b	245	G
10	b	248	G
10	b	252	G
10	b	255	A
10	b	264	C
10	b	265	A
10	b	266	G
10	b	271	G
10	b	278	A
10	b	279	A
10	b	280	U
10	b	281	C
10	b	294	A
10	b	298	G
10	b	300	A
10	b	302	C
10	b	317	G
10	b	318	C
10	b	322	A
10	b	329	G
10	b	330	A
10	b	331	C
10	b	332	A
10	b	343	C
10	b	345	A
10	b	346	A
10	b	347	A
10	b	352	A
10	b	353	C
10	b	355	U
10	b	358	U
10	b	359	G
10	b	362	A
10	b	363	G
10	b	366	C
10	b	367	G
10	b	371	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	372	G
10	b	373	U
10	b	386	G
10	b	387	U
10	b	390	U
10	b	391	A
10	b	395	U
10	b	396	G
10	b	405	U
10	b	406	G
10	b	417	C
10	b	418	C
10	b	439	A
10	b	442	G
10	b	446	G
10	b	451	U
10	b	457	A
10	b	464	U
10	b	467	G
10	b	471	A
10	b	472	A
10	b	474	G
10	b	481	G
10	b	487	C
10	b	491	G
10	b	501	A
10	b	503	A
10	b	505	A
10	b	507	A
10	b	508	A
10	b	509	C
10	b	510	C
10	b	513	A
10	b	527	C
10	b	529	A
10	b	531	C
10	b	532	A
10	b	538	A
10	b	558	A
10	b	559	C
10	b	565	A
10	b	570	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	575	U
10	b	577	A
10	b	579	G
10	b	590	U
10	b	604	A
10	b	605	A
10	b	606	G
10	b	608	U
10	b	615	A
10	b	616	A
10	b	617	U
10	b	624	G
10	b	629	A
10	b	636	C
10	b	639	A
10	b	642	C
10	b	644	U
10	b	648	U
10	b	649	G
10	b	655	U
10	b	656	A
10	b	657	A
10	b	661	G
10	b	670	A
10	b	671	G
10	b	672	A
10	b	688	U
10	b	704	U
10	b	706	G
10	b	719	C
10	b	720	A
10	b	725	C
10	b	729	A
10	b	732	A
10	b	740	G
10	b	749	U
10	b	750	G
10	b	754	A
10	b	759	G
10	b	764	U
10	b	766	A
10	b	767	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	777	G
10	b	778	G
10	b	784	A
10	b	786	G
10	b	787	G
10	b	791	A
10	b	793	C
10	b	807	G
10	b	808	C
10	b	811	G
10	b	813	U
10	b	814	C
10	b	821	A
10	b	829	U
10	b	832	G
10	b	848	U
10	b	849	U
10	b	858	G
10	b	860	G
10	b	861	G
10	b	868	A
10	b	871	G
10	b	874	U
10	b	875	C
10	b	878	C
10	b	879	A
10	b	880	A
10	b	882	G
10	b	883	G
10	b	884	G
10	b	885	G
10	b	886	U
10	b	889	U
10	b	890	C
10	b	896	U
10	b	897	U
10	b	898	A
10	b	899	C
10	b	902	A
10	b	909	G
10	b	912	A
10	b	913	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	914	C
10	b	921	U
10	b	933	U
10	b	943	A
10	b	947	A
10	b	948	C
10	b	963	C
10	b	975	A
10	b	976	G
10	b	985	A
10	b	991	G
10	b	992	A
10	b	998	A
10	b	1005	G
10	b	1007	C
10	b	1012	A
10	b	1014	U
10	b	1015	C
10	b	1021	U
10	b	1024	G
10	b	1028	G
10	b	1035	U
10	b	1037	U
10	b	1040	G
10	b	1049	G
10	b	1055	C
10	b	1056	A
10	b	1058	G
10	b	1059	A
10	b	1060	U
10	b	1061	G
10	b	1062	U
10	b	1063	U
10	b	1064	G
10	b	1066	C
10	b	1068	U
10	b	1069	A
10	b	1070	G
10	b	1071	A
10	b	1072	A
10	b	1073	G
10	b	1075	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	1076	G
10	b	1077	C
10	b	1078	C
10	b	1079	A
10	b	1080	U
10	b	1081	C
10	b	1082	A
10	b	1083	U
10	b	1086	A
10	b	1087	A
10	b	1088	A
10	b	1089	G
10	b	1090	A
10	b	1091	A
10	b	1092	A
10	b	1097	A
10	b	1099	U
10	b	1100	A
10	b	1101	G
10	b	1102	C
10	b	1103	U
10	b	1104	C
10	b	1106	C
10	b	1107	U
10	b	1108	G
10	b	1111	C
10	b	1113	A
10	b	1114	G
10	b	1119	C
10	b	1121	U
10	b	1132	U
10	b	1134	U
10	b	1135	A
10	b	1136	A
10	b	1137	C
10	b	1138	G
10	b	1144	A
10	b	1170	G
10	b	1171	A
10	b	1172	C
10	b	1173	G
10	b	1174	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	1175	U
10	b	1177	A
10	b	1178	U
10	b	1179	G
10	b	1187	G
10	b	1189	G
10	b	1190	U
10	b	1197	G
10	b	1206	A
10	b	1207	A
10	b	1208	G
10	b	1209	C
10	b	1212	G
10	b	1214	G
10	b	1226	U
10	b	1229	G
10	b	1234	G
10	b	1238	G
10	b	1239	A
10	b	1240	G
10	b	1242	U
10	b	1243	A
10	b	1244	U
10	b	1246	A
10	b	1249	A
10	b	1251	U
10	b	1252	G
10	b	1255	A
10	b	1257	U
10	b	1258	G
10	b	1268	G
10	b	1273	G
10	b	1274	A
10	b	1275	U
10	b	1277	A
10	b	1278	A
10	b	1281	G
10	b	1286	A
10	b	1289	A
10	b	1291	C
10	b	1302	G
10	b	1303	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	1304	A
10	b	1313	G
10	b	1321	C
10	b	1323	A
10	b	1328	U
10	b	1331	U
10	b	1336	G
10	b	1342	U
10	b	1346	U
10	b	1354	U
10	b	1361	A
10	b	1367	A
10	b	1370	G
10	b	1380	A
10	b	1381	U
10	b	1382	G
10	b	1385	A
10	b	1388	C
10	b	1397	A
10	b	1398	U
10	b	1402	U
10	b	1412	G
10	b	1413	U
10	b	1417	U
10	b	1418	G
10	b	1421	A
10	b	1422	A
10	b	1423	G
10	b	1429	A
10	b	1430	C
10	b	1444	U
10	b	1453	C
10	b	1454	G
10	b	1455	A
10	b	1456	C
10	b	1457	G
10	b	1461	G
10	b	1462	U
10	b	1463	C
10	b	1469	U
10	b	1471	A
10	b	1473	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	1477	G
10	b	1478	U
10	b	1479	A
10	b	1480	G
10	b	1484	G
10	b	1495	C
10	b	1497	A
10	b	1498	A
10	b	1499	U
10	b	1500	C
10	b	1505	A
10	b	1507	A
10	b	1510	A
10	b	1511	A
10	b	1525	U
10	b	1526	G
10	b	1531	G
10	b	1534	A
10	b	1535	C
10	b	1538	C
10	b	1539	G
10	b	1540	G
10	b	1541	U
10	b	1542	G
10	b	1544	U
10	b	1545	G
10	b	1549	C
10	b	1554	A
10	b	1556	U
10	b	1558	C
10	b	1561	U
10	b	1567	C
10	b	1568	A
10	b	1570	G
10	b	1571	A
10	b	1580	U
10	b	1583	G
10	b	1585	A
10	b	1586	U
10	b	1587	C
10	b	1598	A
10	b	1601	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	1609	C
10	b	1610	A
10	b	1612	A
10	b	1620	A
10	b	1621	G
10	b	1649	U
10	b	1650	U
10	b	1651	G
10	b	1662	G
10	b	1670	A
10	b	1676	G
10	b	1677	C
10	b	1680	A
10	b	1697	G
10	b	1705	G
10	b	1707	A
10	b	1708	C
10	b	1709	G
10	b	1717	G
10	b	1720	G
10	b	1723	G
10	b	1724	A
10	b	1732	C
10	b	1733	G
10	b	1735	G
10	b	1736	G
10	b	1740	G
10	b	1750	C
10	b	1758	G
10	b	1759	A
10	b	1760	U
10	b	1765	G
10	b	1766	C
10	b	1775	A
10	b	1778	G
10	b	1783	U
10	b	1784	U
10	b	1786	A
10	b	1788	A
10	b	1793	A
10	b	1802	C
10	b	1803	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	1810	A
10	b	1813	G
10	b	1818	C
10	b	1831	A
10	b	1835	C
10	b	1844	G
10	b	1851	G
10	b	1859	G
10	b	1864	G
10	b	1870	C
10	b	1886	U
10	b	1888	G
10	b	1899	C
10	b	1910	G
10	b	1911	G
10	b	1912	C
10	b	1914	G
10	b	1917	A
10	b	1918	C
10	b	1922	A
10	b	1924	C
10	b	1931	A
10	b	1933	G
10	b	1934	G
10	b	1935	U
10	b	1941	A
10	b	1942	A
10	b	1944	U
10	b	1959	U
10	b	1971	C
10	b	1974	A
10	b	1975	U
10	b	1976	G
10	b	1978	C
10	b	1979	G
10	b	1985	A
10	b	1986	U
10	b	1995	U
10	b	1996	G
10	b	1997	U
10	b	2001	C
10	b	2024	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	2027	C
10	b	2034	A
10	b	2035	A
10	b	2036	G
10	b	2037	A
10	b	2039	G
10	b	2040	C
10	b	2047	C
10	b	2053	G
10	b	2059	C
10	b	2060	G
10	b	2064	A
10	b	2065	G
10	b	2066	A
10	b	2067	C
10	b	2071	G
10	b	2073	G
10	b	2081	A
10	b	2084	A
10	b	2097	G
10	b	2102	U
10	b	2103	U
10	b	2105	A
10	b	2109	U
10	b	2111	G
10	b	2112	A
10	b	2113	U
10	b	2115	U
10	b	2116	G
10	b	2119	G
10	b	2120	G
10	b	2121	A
10	b	2122	U
10	b	2124	G
10	b	2125	G
10	b	2126	U
10	b	2127	G
10	b	2128	G
10	b	2129	G
10	b	2131	G
10	b	2132	G
10	b	2134	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	2136	U
10	b	2139	A
10	b	2140	G
10	b	2142	G
10	b	2146	A
10	b	2149	C
10	b	2150	C
10	b	2151	A
10	b	2152	G
10	b	2153	U
10	b	2155	U
10	b	2156	G
10	b	2159	U
10	b	2160	G
10	b	2162	A
10	b	2163	G
10	b	2164	C
10	b	2166	G
10	b	2167	G
10	b	2168	C
10	b	2169	C
10	b	2170	U
10	b	2172	G
10	b	2173	A
10	b	2174	A
10	b	2176	U
10	b	2177	A
10	b	2179	C
10	b	2180	A
10	b	2181	C
10	b	2183	C
10	b	2185	U
10	b	2186	U
10	b	2189	U
10	b	2191	U
10	b	2192	U
10	b	2196	U
10	b	2202	A
10	b	2203	A
10	b	2207	U
10	b	2208	G
10	b	2215	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	2216	A
10	b	2217	U
10	b	2218	C
10	b	2229	A
10	b	2233	U
10	b	2242	G
10	b	2243	G
10	b	2247	U
10	b	2272	A
10	b	2275	G
10	b	2283	G
10	b	2284	G
10	b	2287	C
10	b	2291	A
10	b	2292	A
10	b	2300	U
10	b	2309	U
10	b	2310	C
10	b	2312	G
10	b	2313	A
10	b	2315	A
10	b	2316	U
10	b	2326	A
10	b	2329	G
10	b	2334	G
10	b	2335	G
10	b	2337	A
10	b	2338	U
10	b	2339	A
10	b	2340	A
10	b	2349	G
10	b	2351	C
10	b	2352	U
10	b	2354	C
10	b	2358	C
10	b	2361	G
10	b	2365	G
10	b	2379	G
10	b	2380	A
10	b	2381	A
10	b	2383	G
10	b	2384	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	2385	A
10	b	2387	G
10	b	2388	U
10	b	2389	C
10	b	2393	G
10	b	2395	G
10	b	2406	U
10	b	2408	U
10	b	2409	G
10	b	2410	A
10	b	2411	A
10	b	2417	G
10	b	2426	C
10	b	2427	U
10	b	2429	A
10	b	2430	A
10	b	2433	G
10	b	2434	A
10	b	2438	A
10	b	2445	U
10	b	2451	G
10	b	2452	A
10	b	2461	U
10	b	2463	A
10	b	2478	U
10	b	2480	A
10	b	2482	A
10	b	2488	G
10	b	2490	C
10	b	2494	G
10	b	2498	G
10	b	2501	A
10	b	2506	G
10	b	2508	U
10	b	2509	G
10	b	2510	U
10	b	2521	C
10	b	2522	A
10	b	2533	G
10	b	2539	G
10	b	2540	G
10	b	2551	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	2558	U
10	b	2560	C
10	b	2566	U
10	b	2570	A
10	b	2571	G
10	b	2572	U
10	b	2576	A
10	b	2577	C
10	b	2585	G
10	b	2586	G
10	b	2590	U
10	b	2599	G
10	b	2606	A
10	b	2607	G
10	b	2613	U
10	b	2617	U
10	b	2618	A
10	b	2619	U
10	b	2627	G
10	b	2633	U
10	b	2645	G
10	b	2650	C
10	b	2653	C
10	b	2654	U
10	b	2659	G
10	b	2663	G
10	b	2664	A
10	b	2665	G
10	b	2667	G
10	b	2673	G
10	b	2677	G
10	b	2686	A
10	b	2688	U
10	b	2689	G
10	b	2693	U
10	b	2703	C
10	b	2711	U
10	b	2718	G
10	b	2720	C
10	b	2730	A
10	b	2732	U
10	b	2736	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	2737	A
10	b	2740	A
10	b	2742	A
10	b	2748	G
10	b	2752	A
10	b	2755	G
10	b	2756	C
10	b	2757	A
10	b	2762	A
10	b	2765	A
10	b	2766	C
10	b	2769	A
10	b	2781	G
10	b	2782	A
10	b	2783	U
10	b	2786	G
10	b	2795	G
10	b	2797	C
10	b	2800	C
10	b	2801	U
10	b	2802	U
10	b	2803	G
10	b	2804	A
10	b	2812	G
10	b	2813	A
10	b	2815	G
10	b	2822	U
10	b	2824	A
10	b	2825	A
10	b	2837	U
10	b	2839	A
10	b	2852	G
10	b	2854	A
10	b	2865	U
10	b	2869	U
10	b	2870	U
10	b	2871	G
10	b	2877	A
10	b	2881	G
10	b	2883	A
10	b	2884	C
10	b	2887	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	2888	U
10	b	2889	G
10	b	2890	A
10	b	2897	A
10	b	2898	G
10	b	2899	G
10	b	2905	C
29	v	3	G
29	v	5	G
29	v	6	C
29	v	7	A
29	v	8	U
29	v	9	C
29	v	15	A
29	v	16	U
29	v	17	G
29	v	18	G
29	v	20	U
29	v	25	C
29	v	26	C
29	v	27	U
29	v	34	U
29	v	35	C
29	v	36	C
29	v	38	A
29	v	42	G
29	v	45	G
29	v	46	A
29	v	47	U
29	v	48	G
29	v	49	C
29	v	50	G
29	v	52	G
29	v	54	U
29	v	60	C
29	v	62	C
29	v	63	G
29	v	64	C
29	v	65	U
29	v	67	C
29	v	68	C
29	v	70	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	v	71	C
29	v	75	A

There are no RNA pucker outliers to report.

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.

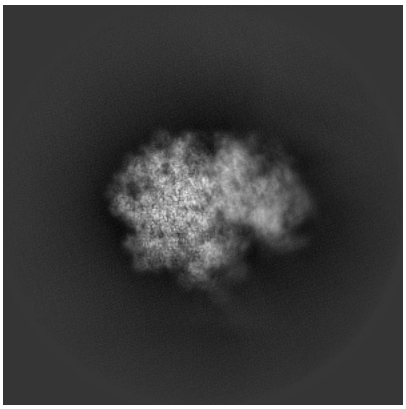
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10891. These allow visual inspection of the internal detail of the map and identification of artifacts.

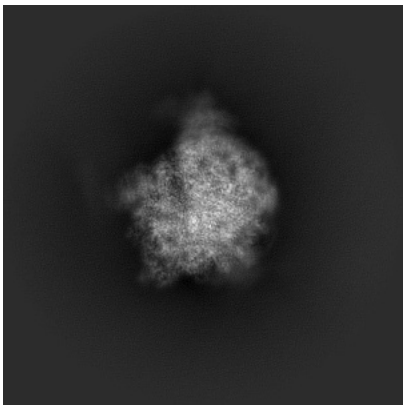
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

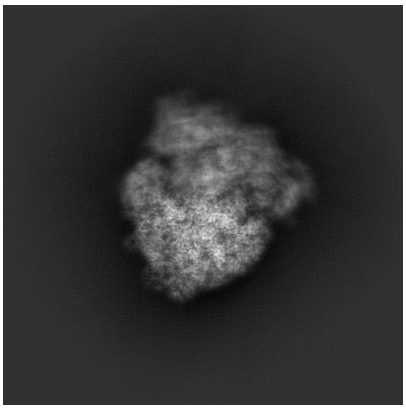
6.1.1 Primary map



X

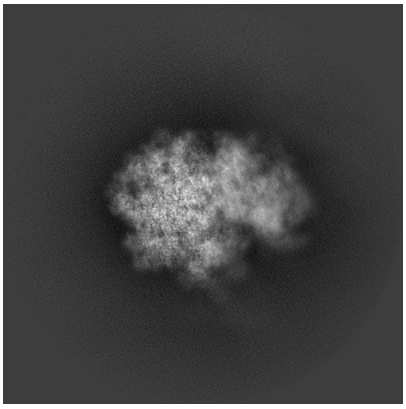


Y

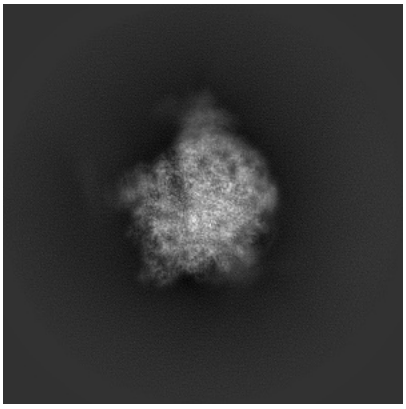


Z

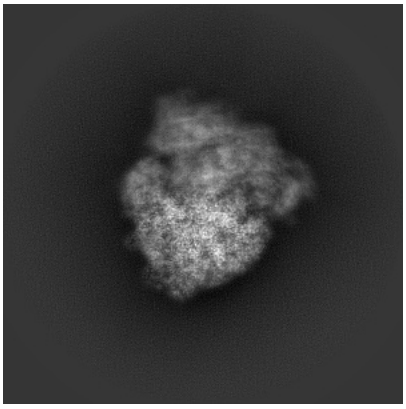
6.1.2 Raw map



X



Y

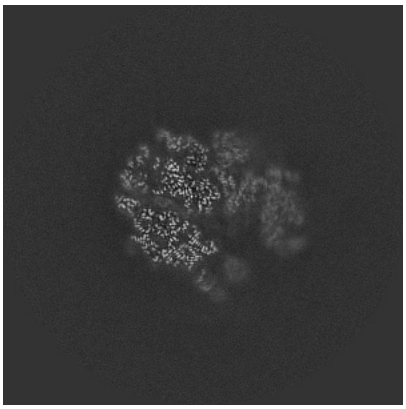


Z

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

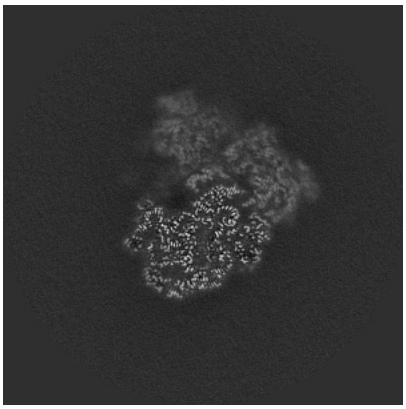
6.2 Central slices (i)

6.2.1 Primary map



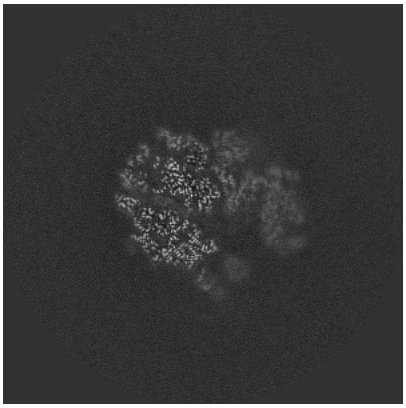
X Index: 240

Y Index: 240

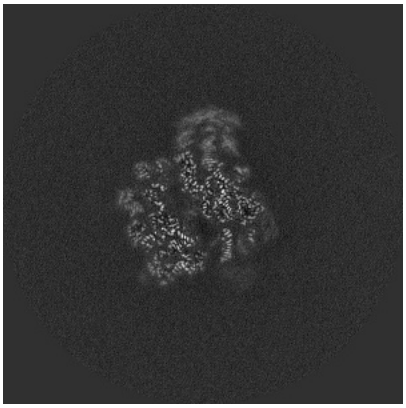


Z Index: 240

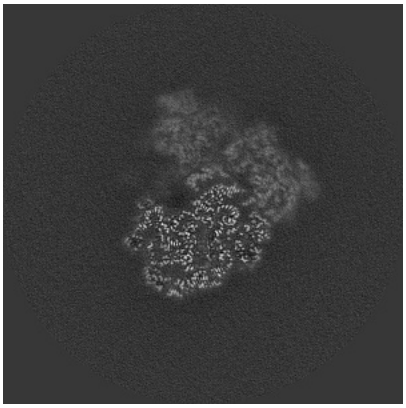
6.2.2 Raw map



X Index: 240



Y Index: 240

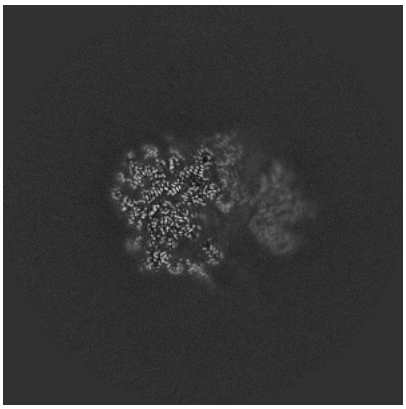


Z Index: 240

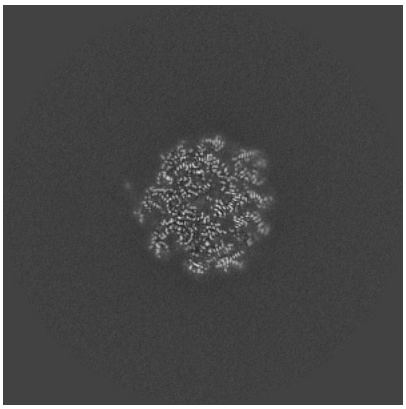
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

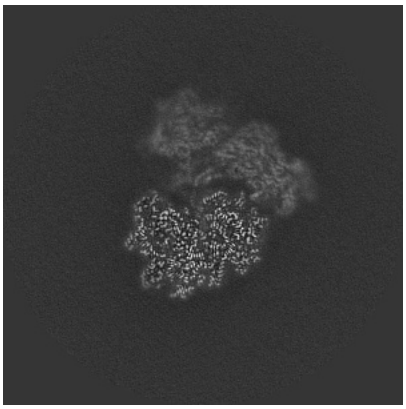
6.3.1 Primary map



X Index: 230

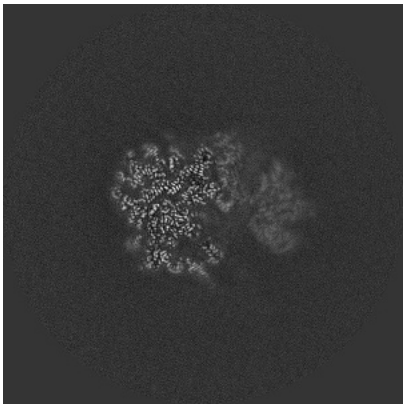


Y Index: 208

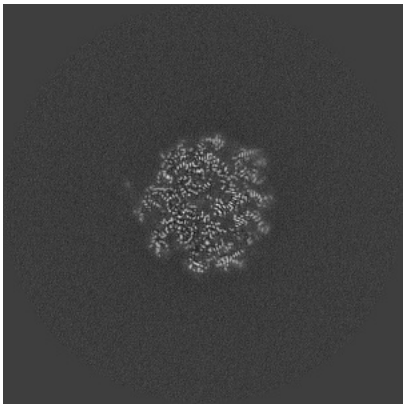


Z Index: 231

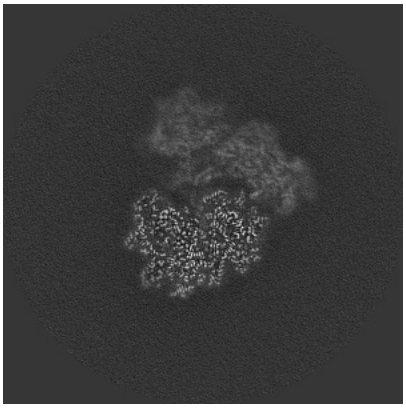
6.3.2 Raw map



X Index: 230



Y Index: 208



Z Index: 231

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

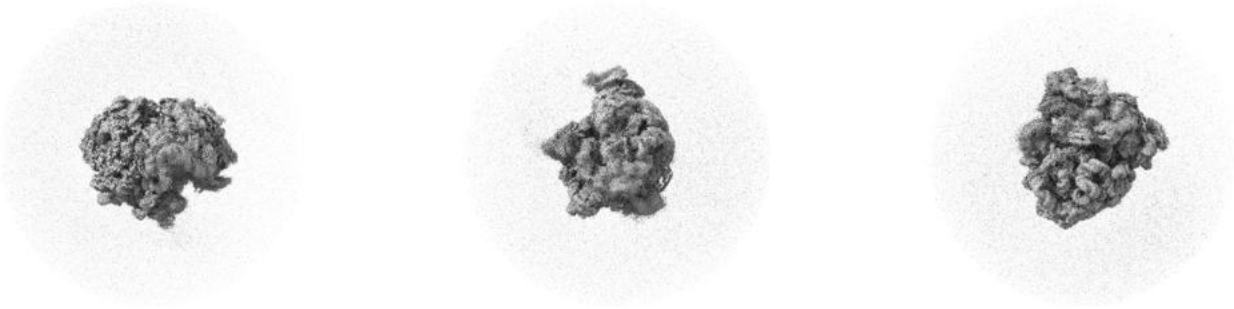
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00741. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

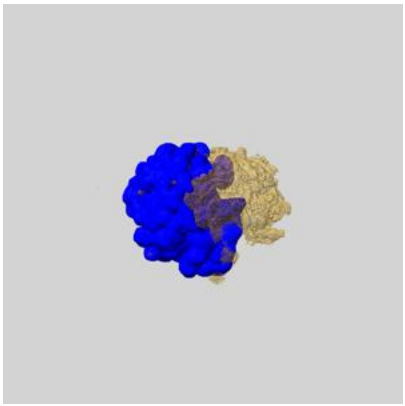
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

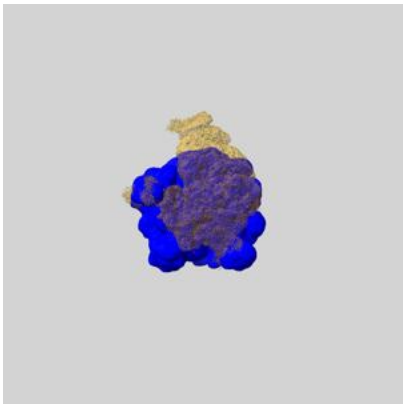
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

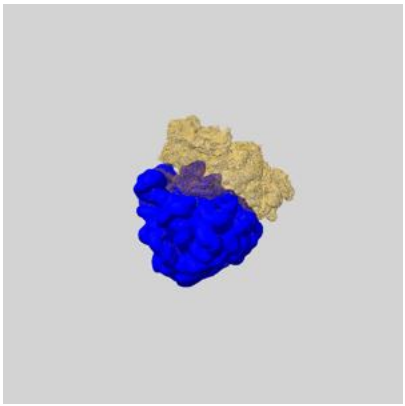
6.5.1 emd_10891_msk_1.map (i)



X



Y

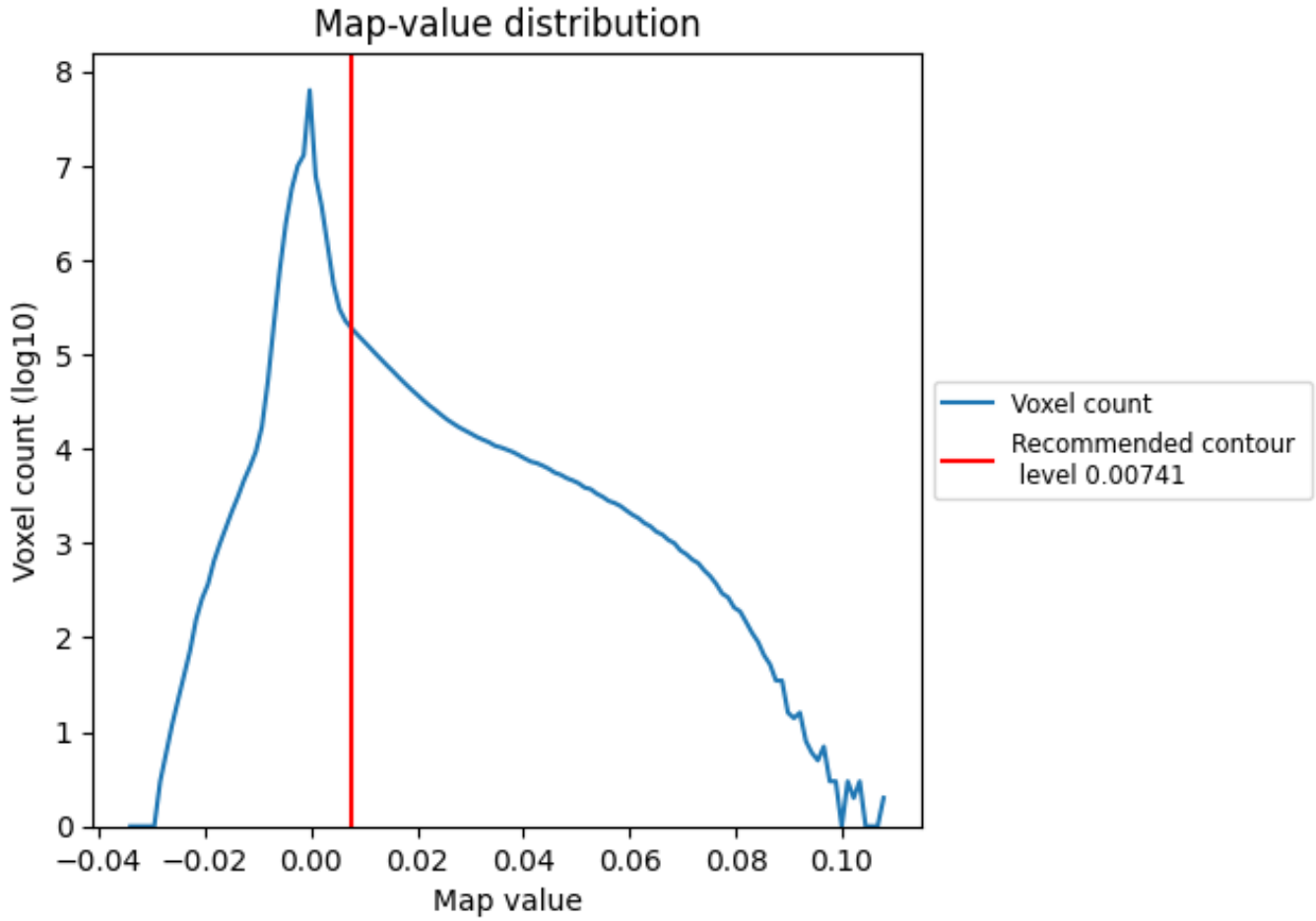


Z

7 Map analysis

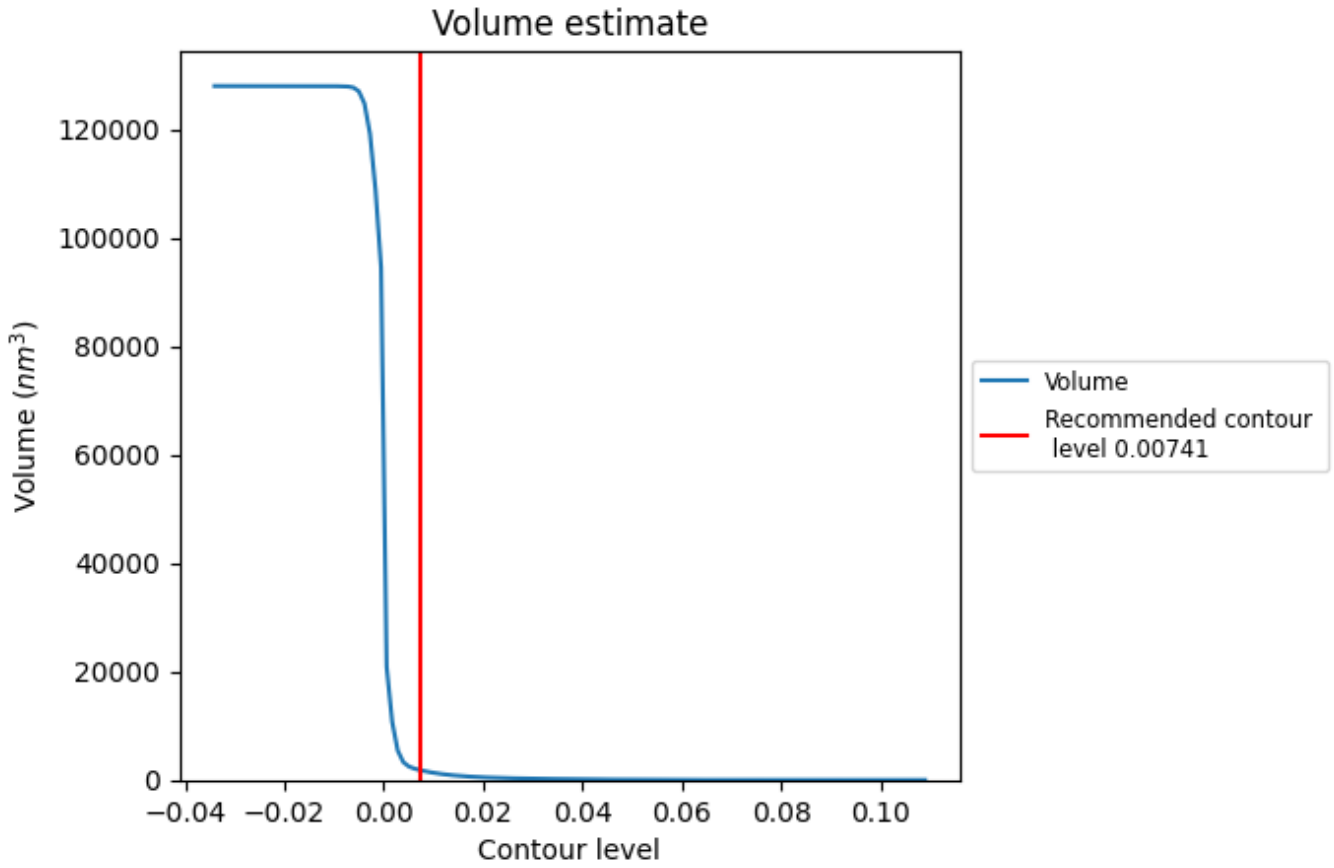
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

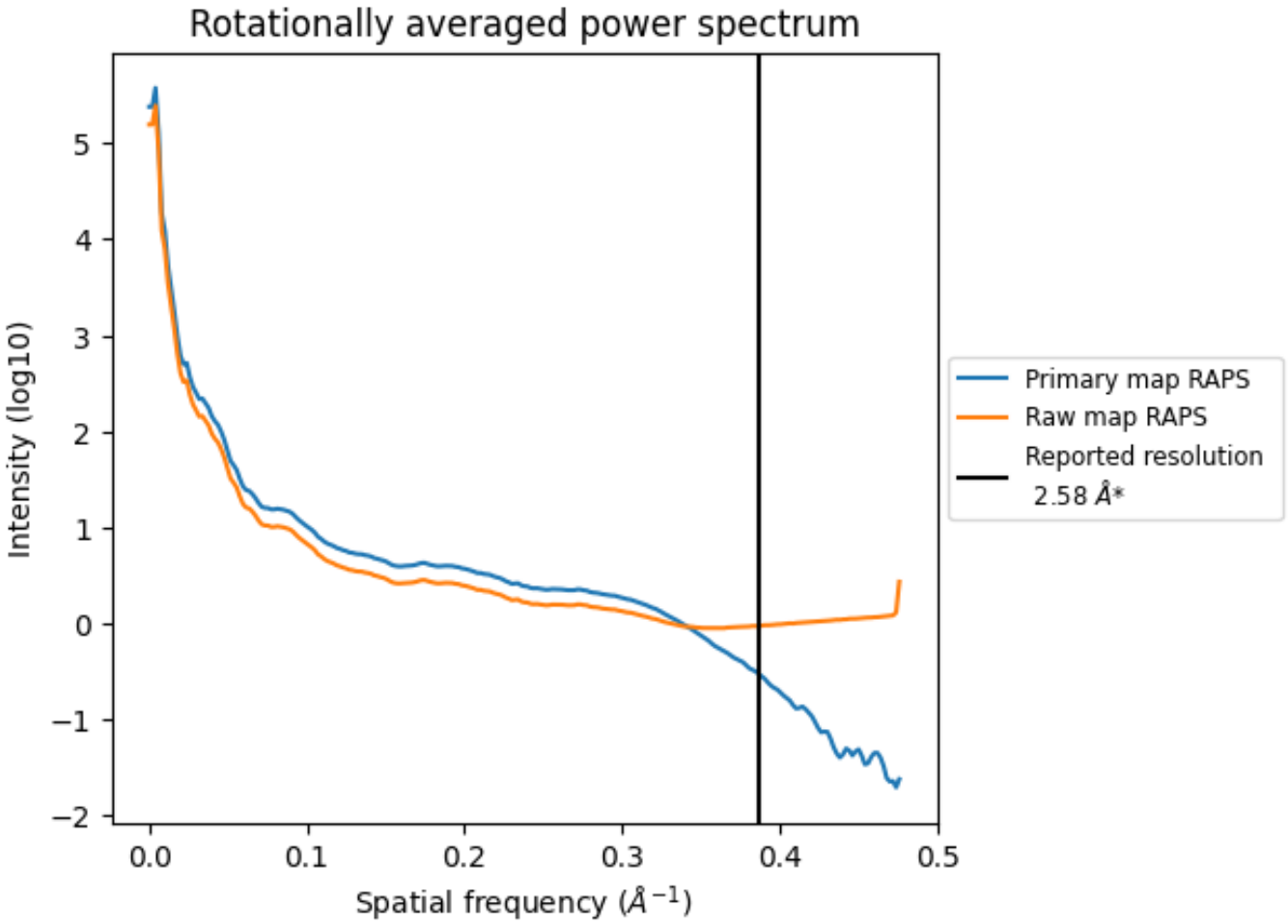
7.2 Volume estimate



The volume at the recommended contour level is 1796 nm^3; this corresponds to an approximate mass of 1623 kDa.

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

7.3 Rotationally averaged power spectrum (i)

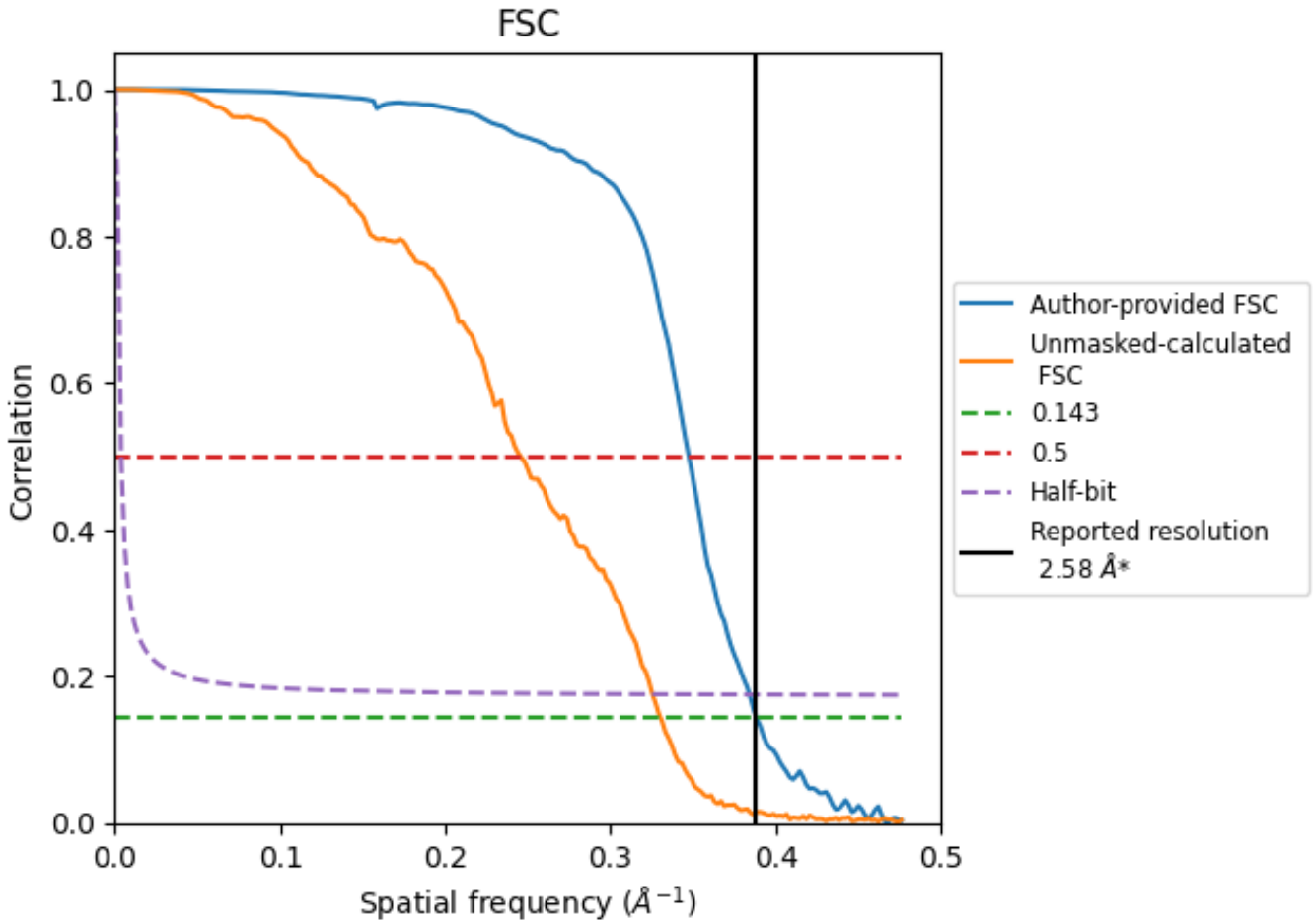


*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.388 $Å^{-1}$

8.2 Resolution estimates (i)

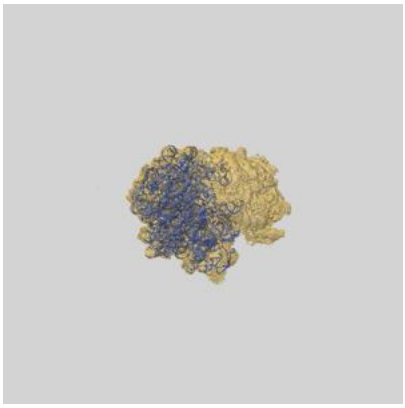
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.57	2.88	2.60
Unmasked-calculated*	3.03	4.07	3.07

*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 3.03 differs from the reported value 2.58 by more than 10 %

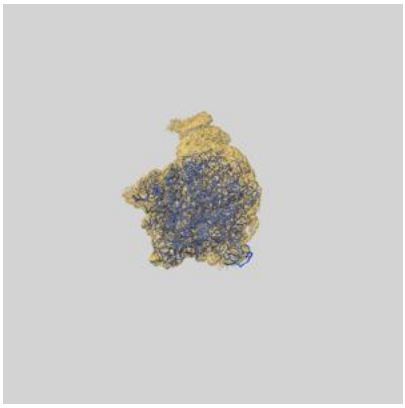
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10891 and PDB model 6YS3. Per-residue inclusion information can be found in section 3 on page 10.

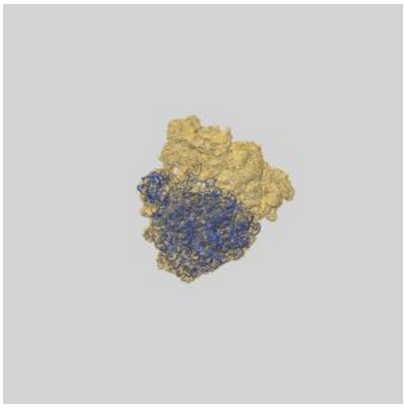
9.1 Map-model overlay



X



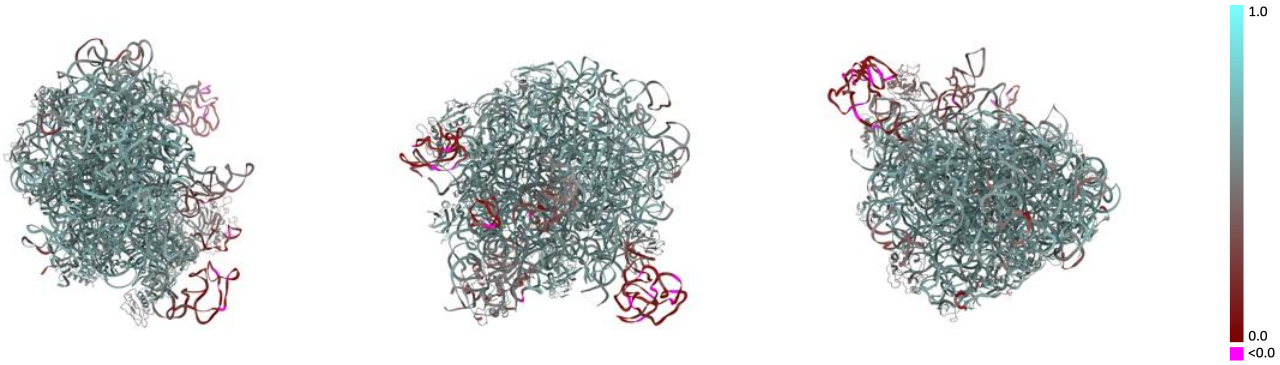
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00741 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.

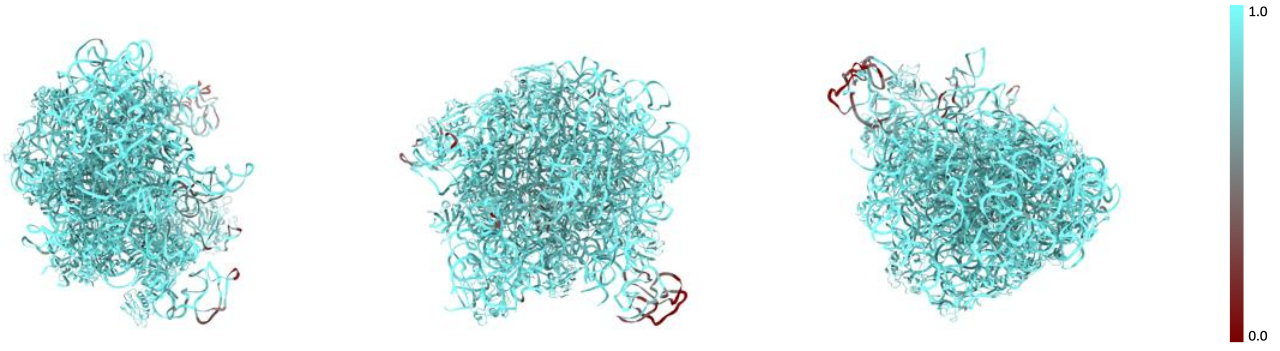
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

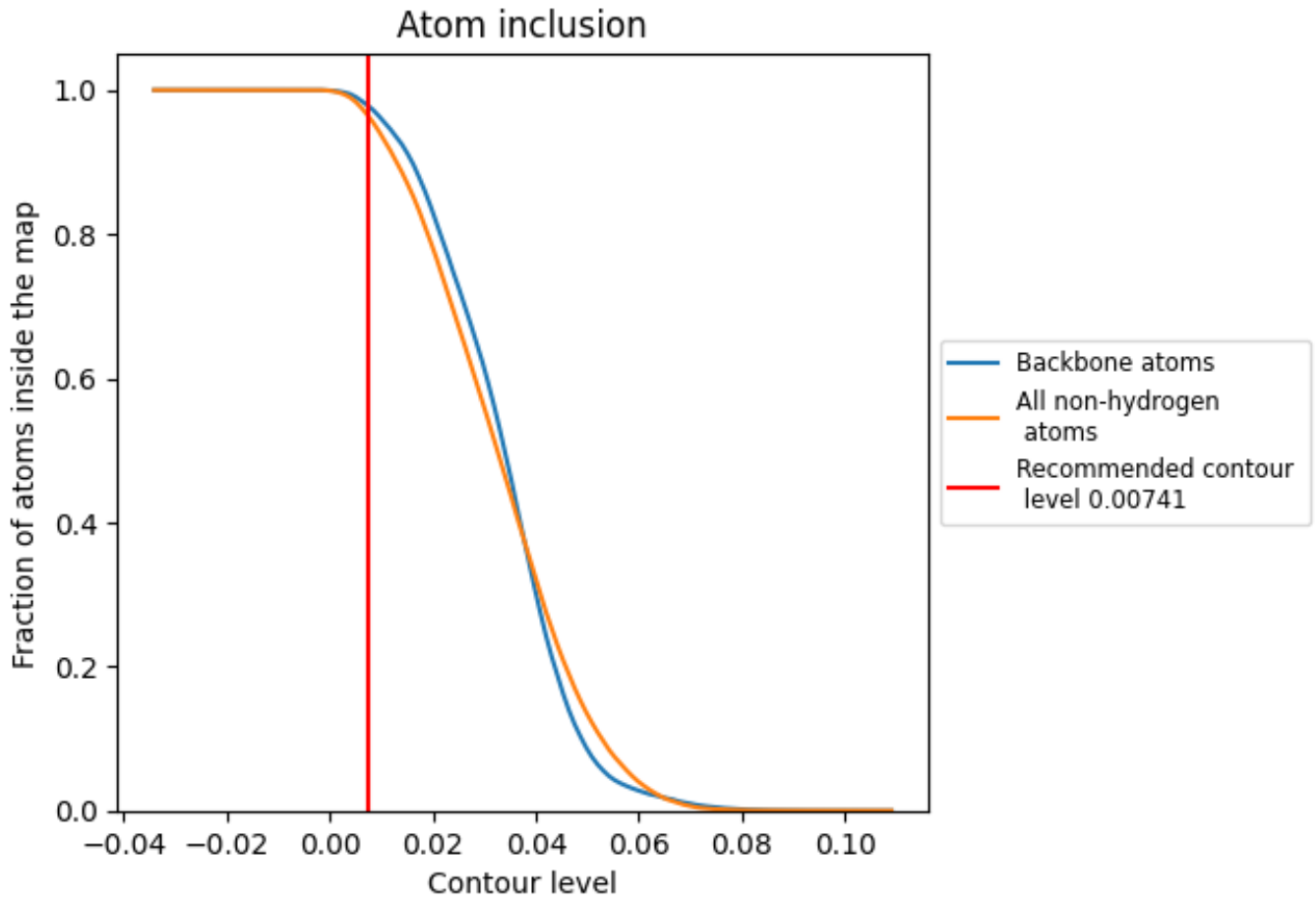
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00741).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00741) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9645	0.5680
0	0.9684	0.5890
1	0.9255	0.5280
2	0.9625	0.5880
3	0.9833	0.6010
4	0.9277	0.5590
6	0.9803	0.6240
7	0.9796	0.6330
8	0.9692	0.5930
a	0.9873	0.5370
b	0.9749	0.5750
c	0.9717	0.6040
d	0.9629	0.6020
e	0.9395	0.5640
f	0.8813	0.3830
g	0.9221	0.4980
h	0.8873	0.4860
j	0.9664	0.6040
k	0.9562	0.5900
l	0.9605	0.5910
m	0.9655	0.6000
n	0.9859	0.6090
o	0.9467	0.4960
p	0.9408	0.5770
q	0.9769	0.6140
r	0.9560	0.5860
s	0.9613	0.6020
t	0.9432	0.5570
u	0.9452	0.5310
v	0.7416	0.3480
w	0.9417	0.5670
y	0.9725	0.6070
z	0.7425	0.3460