Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 10:20 am BST

PDB ID	:	6YST
EMDB ID	:	EMD-10907
Title	:	Structure of the P+9 ArfB-ribosome complex with P/E hybrid tRNA in the post-hydrolysis state
Authors	:	Chan, K.-H.; Petrychenko, V.; Mueller, C.; Maracci, C.; Holtkamp, W.; Wilson, D.N.; Fischer, N.; Rodnina, M.V.
Deposited on	:	2020-04-23
Resolution	:	3.20 Å(reported)
Based on initial models	:	4RB7, 5AFI, 5O2R, 4V95

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.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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 61 unique types of molecules in this entry. The entry contains 146847 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 L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	56	444	269	94	80	1	0	0

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	50	409	263	75	71	0	0

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	5	131	647	385	131	131	0	0

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2903	Total	C	N	O	P	0	0
			62336	27815	11468	20150	2903		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

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

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

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

- Molecule 15 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	I	141	Total	C	N	O	0	0
			693	411	141	141		

- 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
			1045	649	206	189	1		

- 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	114	Total	C	N	O	S	0	0
			917	574	179	163	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	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	110	Total	C	N	O	S	0	0
			857	532	166	156	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 protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	75	Total 575	C 356	N 116	O 102	S 1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	63	Total 509	C 313	N 99	O 95	S 2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	58	Total 449	C 281	N 87	O 79	S 2	0	0

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total 33050	C 14748	N 6057	O 10705	P 1540	0	0

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	36	ALA	-	insertion	UNP I2X5X6

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a protein called Api137.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	v	14	Total 121	C 80	N 25	O 16	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	10	ARG	GLN	conflict	UNP Q8WSY8

- Molecule 56 is a RNA chain called P/E-site tRNAPhe.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	w	76	Total 1631	C 731	N 291	O 531	P 76	S 2	0	0

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	4	Total 82	C 37	N 12	O 29	P 4	0	0

- Molecule 58 is a protein called Alternative stalled-ribosome rescue factor B.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	139	Total 1078	C 666	N 215	O 195	S 2	0	0

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	0	1	Total 1	Mg 1	0
59	4	1	Total 1	Mg 1	0
59	6	1	Total 1	Mg 1	0
59	A	206	Total 206	Mg 206	0
59	B	6	Total 6	Mg 6	0
59	C	1	Total 1	Mg 1	0
59	D	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms	AltConf
59	S	1	Total Mg 1 1	0
59	a	35	Total Mg 35 35	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
60	4	1	Total Zn 1 1	0
60	6	1	Total Zn 1 1	0

- Molecule 61 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
61	A	1	Total Na 1 1	0
61	M	1	Total Na 1 1	0

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

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23340	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2.5	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	14.075	Depositor
Minimum map value	-5.703	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

41 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	$\#\|Z\| > 2$
56	5MU	w	54	56	19,22,23	4.85	7 (36%)	28,32,35	3.61	9 (32%)
56	G7M	w	46	56	20,26,27	2.47	7 (35%)	17,39,42	1.14	1 (5%)
8	OMU	A	2552	8	19,22,23	2.80	8 (42%)	26,31,34	1.82	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	1MG	A	745	8	18,26,27	2.53	4 (22%)	19,39,42	1.51	4 (21%)
34	2MG	a	966	34,56	18,26,27	2.77	7 (38%)	16,38,41	1.34	3 (18%)
8	3TD	A	1915	8	18,22,23	4.25	5 (27%)	22,32,35	1.49	2 (9%)
8	5MU	A	1939	8	19,22,23	4.60	7 (36%)	28,32,35	3.88	10 (35%)
34	4OC	a	1402	34	20,23,24	2.90	8 (40%)	26,32,35	0.94	2 (7%)
56	4SU	w	8	56	18,21,22	3.75	8 (44%)	26,30,33	2.16	5 (19%)
8	2MG	A	2445	8	18,26,27	2.14	4 (22%)	16,38,41	1.94	6 (37%)
8	6MZ	A	1618	8	18,25,26	2.21	4 (22%)	16,36,39	1.62	2 (12%)
8	PSU	A	2457	8	18,21,22	1.06	3 (16%)	22,30,33	2.14	6 (27%)
8	G7M	A	2069	8	20,26,27	3.80	9 (45%)	17,39,42	1.11	1 (5%)
34	5MC	a	967	34	18,22,23	3.72	7 (38%)	26,32,35	1.09	1 (3%)
8	PSU	A	2604	8	18,21,22	1.10	2 (11%)	22,30,33	1.95	5 (22%)
56	PSU	w	39	56	18,21,22	1.01	1 (5%)	22,30,33	1.73	3 (13%)
34	MA6	a	1518	34	18,26,27	1.05	1 (5%)	19,38,41	2.70	2 (10%)
34	5MC	a	1407	34	18,22,23	3.54	7 (38%)	26,32,35	1.15	2 (7%)
34	2MG	a	1207	34	18,26,27	2.63	7 (38%)	16,38,41	1.36	3 (18%)
56	PSU	w	55	56	18,21,22	1.08	1 (5%)	22,30,33	1.80	4 (18%)
8	PSU	A	2504	8	18,21,22	1.05	3 (16%)	22,30,33	1.71	4 (18%)
8	2MA	A	2503	59,8	17,25,26	2.33	5 (29%)	17,37,40	1.41	3 (17%)
8	PSU	A	746	8	18,21,22	1.07	2 (11%)	22,30,33	1.84	4 (18%)
34	G7M	a	527	34	20,26,27	3.93	9 (45%)	17,39,42	0.99	1 (5%)
8	PSU	A	1917	8	18,21,22	1.11	3 (16%)	22,30,33	1.93	5 (22%)
56	MIA	w	37	34,56	24,31,32	2.58	4 (16%)	26,44,47	4.24	8 (30%)
8	OMG	A	2251	8	18,26,27	2.45	8 (44%)	19,38,41	1.51	4 (21%)
8	PSU	A	2605	8	18,21,22	1.12	2 (11%)	22,30,33	1.80	4 (18%)
8	2MG	A	1835	8	18,26,27	2.48	7 (38%)	16,38,41	1.52	4 (25%)
8	OMC	A	2498	59,8	19,22,23	2.74	7 (36%)	26,31,34	0.77	0
8	5MC	A	1962	8	18,22,23	3.58	7 (38%)	26,32,35	1.17	2 (7%)
34	UR3	a	1498	34,59	19,22,23	2.74	7 (36%)	26,32,35	1.50	4 (15%)
34	MA6	a	1519	34	18,26,27	1.02	1 (5%)	19,38,41	2.57	2 (10%)
56	PSU	w	32	56	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
34	PSU	a	516	34	18,21,22	0.88	1 (5%)	22,30,33	1.67	5 (22%)
8	PSU	A	1911	8	18,21,22	1.07	2 (11%)	22,30,33	1.87	4 (18%)
8	PSU	A	955	8	18,21,22	1.14	2 (11%)	22,30,33	1.88	4 (18%)
8	6MZ	A	2030	8	18,25,26	2.12	4 (22%)	16,36,39	2.51	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	5MC	A	747	8	18,22,23	3.52	7 (38%)	26,32,35	1.16	2 (7%)
34	2MG	a	1516	34	18,26,27	2.63	7 (38%)	16,38,41	1.51	4 (25%)
8	PSU	A	2580	8	18,21,22	1.18	3 (16%)	22,30,33	2.07	6 (27%)

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
56	5MU	w	54	56	-	0/7/25/26	0/2/2/2
56	G7M	w	46	56	-	3/3/25/26	0/3/3/3
8	OMU	A	2552	8	-	5/9/27/28	0/2/2/2
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
34	2MG	a	966	34,56	-	2/5/27/28	0/3/3/3
8	3TD	A	1915	8	-	3/7/25/26	0/2/2/2
8	5MU	A	1939	8	-	0/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	0/9/29/30	0/2/2/2
56	4SU	w	8	56	-	0/7/25/26	0/2/2/2
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
8	6MZ	A	1618	8	-	2/5/27/28	0/3/3/3
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
34	5MC	a	967	34	-	4/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	3/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	3/7/29/30	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	3/5/27/28	0/3/3/3
56	PSU	w	55	56	-	1/7/25/26	0/2/2/2
8	PSU	A	2504	8	-	2/7/25/26	0/2/2/2
8	2MA	A	2503	59,8	-	2/3/25/26	0/3/3/3
8	PSU	A	746	8	-	4/7/25/26	0/2/2/2
34	G7M	a	527	34	-	1/3/25/26	0/3/3/3
8	PSU	A	1917	8	-	0/7/25/26	0/2/2/2
56	MIA	w	37	34,56	-	8/11/33/34	0/3/3/3
8	OMG	A	2251	8	-	1/5/27/28	0/3/3/3
8	PSU	A	2605	8	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	OMC	A	2498	59,8	-	2/9/27/28	0/2/2/2
8	5MC	A	1962	8	-	0/7/25/26	0/2/2/2
34	UR3	a	1498	34,59	-	6/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	0/7/29/30	0/3/3/3
56	PSU	w	32	56	-	5/7/25/26	0/2/2/2
34	PSU	a	516	34	-	2/7/25/26	0/2/2/2
8	PSU	A	1911	8	-	1/7/25/26	0/2/2/2
8	PSU	A	955	8	-	3/7/25/26	0/2/2/2
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3
8	5MC	A	747	8	-	3/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2

All (199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1915	3TD	C6-C5	12.78	1.50	1.35
56	w	54	5MU	C2-N1	11.06	1.56	1.38
56	w	54	5MU	C6-N1	10.58	1.56	1.38
8	A	1939	5MU	C6-N1	10.09	1.55	1.38
56	w	54	5MU	C4-C5	10.00	1.61	1.44
34	a	527	G7M	C8-N7	9.76	1.50	1.33
8	A	1939	5MU	C2-N1	9.48	1.53	1.38
34	a	967	5MC	C6-C5	9.47	1.50	1.34
8	A	2069	G7M	C8-N7	9.46	1.50	1.33
8	A	1915	3TD	C2-N1	9.39	1.49	1.37
34	a	527	G7M	C8-N9	9.34	1.50	1.33
8	A	2069	G7M	C8-N9	9.20	1.50	1.33
8	A	1939	5MU	C4-C5	9.15	1.60	1.44
34	a	1407	5MC	C6-C5	8.89	1.49	1.34
8	A	1962	5MC	C6-C5	8.83	1.49	1.34
56	w	8	4SU	C4-N3	8.78	1.47	1.37
8	A	747	5MC	C6-C5	8.74	1.49	1.34
8	A	1939	5MU	C4-N3	-8.56	1.22	1.38
56	w	54	5MU	C4-N3	-7.88	1.24	1.38
56	w	37	MIA	C2-S10	7.73	1.82	1.75
8	A	1618	6MZ	C6-N6	7.70	1.47	1.35
56	w	8	4SU	C2-N1	7.68	1.50	1.38
34	a	1498	UR3	C2-N1	7.20	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2030	6MZ	C6-N6	7.12	1.46	1.35
56	w	37	MIA	C13-C14	7.06	1.52	1.32
34	a	966	2MG	C2-N2	6.99	1.49	1.33
8	A	745	1MG	C2-N2	6.86	1.46	1.34
8	A	1962	5MC	C4-N3	6.78	1.45	1.34
8	A	2503	2MA	C2-N3	6.76	1.45	1.31
34	a	967	5MC	C4-N3	6.76	1.45	1.34
34	a	1407	5MC	C4-N3	6.59	1.45	1.34
34	a	1402	4OC	C4-N3	6.59	1.44	1.32
8	A	747	5MC	C4-N3	6.58	1.45	1.34
34	a	1207	2MG	C2-N2	6.44	1.47	1.33
8	A	2552	OMU	C2-N3	6.20	1.49	1.38
34	a	1516	2MG	C2-N2	6.19	1.47	1.33
34	a	1498	UR3	C6-C5	6.17	1.49	1.35
34	a	967	5MC	C2-N3	6.14	1.48	1.36
8	A	2552	OMU	C2-N1	6.11	1.48	1.38
8	A	1962	5MC	C2-N3	6.10	1.48	1.36
8	A	2498	OMC	C6-C5	6.02	1.49	1.35
56	w	8	4SU	C6-C5	5.97	1.48	1.35
8	A	747	5MC	C2-N3	5.94	1.48	1.36
8	A	1835	2MG	C2-N2	5.92	1.46	1.33
56	w	8	4SU	C2-N3	5.89	1.48	1.38
34	a	1402	4OC	C6-C5	5.89	1.48	1.35
56	w	54	5MU	C6-C5	5.84	1.44	1.34
34	a	1407	5MC	C2-N3	5.82	1.48	1.36
8	A	1915	3TD	C6-N1	5.81	1.45	1.36
8	A	2498	OMC	C2-N3	5.76	1.48	1.36
34	a	527	G7M	C2-N3	5.76	1.47	1.33
56	w	37	MIA	C6-N6	5.66	1.44	1.34
8	A	1939	5MU	C6-C5	5.61	1.43	1.34
56	w	46	G7M	C2-N3	5.53	1.46	1.33
8	A	2445	2MG	C2'-C1'	-5.52	1.45	1.53
8	A	2552	OMU	C6-C5	5.47	1.47	1.35
34	a	1402	4OC	C2-N3	5.43	1.47	1.36
8	A	2069	G7M	C2-N3	5.27	1.46	1.33
8	A	2498	OMC	C4-N3	5.24	1.45	1.34
34	a	966	2MG	C2-N1	5.18	1.45	1.36
8	A	745	1MG	C2-N3	5.18	1.43	1.34
8	A	2445	2MG	C6-N1	-5.17	1.30	1.37
8	A	2251	OMG	C2-N3	5.12	1.45	1.33
56	w	8	4SU	C4-S4	-5.06	1.58	1.68
34	a	1516	2MG	C4-N3	5.04	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1207	2MG	C4-N3	5.01	1.49	1.37
56	w	46	G7M	C4-N3	4.94	1.49	1.37
34	a	966	2MG	C4-N3	4.94	1.49	1.37
8	A	2251	OMG	C4-N3	4.81	1.49	1.37
34	a	967	5MC	C4-N4	4.79	1.46	1.34
8	A	1835	2MG	C4-N3	4.79	1.49	1.37
34	a	1407	5MC	C4-N4	4.78	1.46	1.34
8	A	747	5MC	C4-N4	4.77	1.46	1.34
34	a	527	G7M	C2-N2	4.75	1.45	1.34
34	a	1498	UR3	C2-N3	4.73	1.48	1.39
8	A	1962	5MC	C4-N4	4.72	1.46	1.34
34	a	527	G7M	C6-N1	4.66	1.44	1.37
8	A	1915	3TD	C2-N3	4.64	1.48	1.38
8	A	2503	2MA	C4-N3	4.60	1.48	1.37
8	A	2069	G7M	C2-N2	4.59	1.45	1.34
8	A	745	1MG	C4-N3	4.53	1.48	1.37
34	a	967	5MC	C6-N1	4.49	1.45	1.38
34	a	1207	2MG	C2-N1	4.45	1.43	1.36
8	A	2069	G7M	C6-N1	4.41	1.44	1.37
8	A	2251	OMG	C2-N2	4.40	1.44	1.34
56	w	46	G7M	C2-N2	4.39	1.44	1.34
34	a	1516	2MG	C2-N1	4.37	1.43	1.36
34	a	967	5MC	C2-N1	4.32	1.49	1.40
34	a	1407	5MC	C6-N1	4.15	1.45	1.38
8	A	1962	5MC	C6-N1	4.13	1.45	1.38
34	a	527	G7M	C4-N3	4.03	1.47	1.37
56	w	46	G7M	C6-N1	4.01	1.43	1.37
8	A	747	5MC	C6-N1	3.99	1.44	1.38
8	A	1835	2MG	C2-N1	3.92	1.43	1.36
34	a	1402	4OC	C4-N4	3.89	1.43	1.35
8	A	1962	5MC	C2-N1	3.88	1.48	1.40
8	A	747	5MC	C2-N1	3.77	1.48	1.40
34	a	1407	5MC	C2-N1	3.75	1.48	1.40
8	A	2069	G7M	C4-N3	3.70	1.46	1.37
56	w	55	PSU	C6-C5	3.66	1.39	1.35
34	a	1402	4OC	C5-C4	3.63	1.48	1.40
8	A	2498	OMC	C4-N4	3.59	1.42	1.33
34	a	527	G7M	C2-N1	3.57	1.46	1.37
8	A	2552	OMU	C4-N3	3.52	1.44	1.38
34	a	1402	4OC	C2-N1	3.48	1.47	1.40
8	A	2069	G7M	C2-N1	3.46	1.46	1.37
8	A	1962	5MC	O2-C2	-3.46	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	747	5MC	O2-C2	-3.43	1.17	1.23
8	A	2445	2MG	C2-N1	-3.39	1.31	1.36
56	w	32	PSU	C6-C5	3.36	1.39	1.35
34	a	1407	5MC	O2-C2	-3.34	1.17	1.23
56	w	46	G7M	C5-C6	3.34	1.54	1.45
8	A	2030	6MZ	C5-C4	-3.34	1.32	1.40
8	A	1835	2MG	O6-C6	-3.33	1.16	1.23
34	a	1516	2MG	C6-N1	3.27	1.42	1.37
56	w	8	4SU	C5-C4	3.25	1.46	1.42
34	a	1207	2MG	C6-N1	3.24	1.42	1.37
34	a	967	5MC	O2-C2	-3.23	1.17	1.23
8	A	1835	2MG	C5-C4	-3.22	1.34	1.43
8	A	2251	OMG	C6-N1	3.17	1.42	1.37
8	A	2498	OMC	O2-C2	-3.15	1.17	1.23
8	A	1939	5MU	O2-C2	-3.15	1.17	1.23
8	A	745	1MG	C5-C4	-3.14	1.35	1.43
34	a	966	2MG	C6-N1	3.13	1.42	1.37
8	A	1917	PSU	C6-C5	3.11	1.38	1.35
34	a	1402	4OC	O2-C2	-3.11	1.17	1.23
34	a	1516	2MG	O6-C6	-3.11	1.17	1.23
8	A	2498	OMC	C2-N1	3.10	1.46	1.40
8	A	2498	OMC	C6-N1	3.08	1.45	1.38
8	A	1939	5MU	O4-C4	-3.05	1.17	1.23
34	a	966	2MG	O6-C6	-3.02	1.17	1.23
34	a	1516	2MG	C5-C4	-3.02	1.35	1.43
8	A	2552	OMU	O4-C4	-3.01	1.18	1.24
8	A	2503	2MA	C5-C4	-3.00	1.35	1.43
8	A	2605	PSU	C6-C5	2.96	1.38	1.35
8	A	1618	6MZ	C5-C4	-2.96	1.33	1.40
56	w	39	PSU	C6-C5	2.96	1.38	1.35
34	a	1516	2MG	C5-C6	2.95	1.53	1.47
8	A	1835	2MG	C6-N1	2.94	1.42	1.37
8	A	1911	PSU	C6-C5	2.94	1.38	1.35
34	a	1207	2MG	C5-C4	-2.93	1.35	1.43
8	A	2552	OMU	O2-C2	-2.90	1.17	1.23
34	a	1207	2MG	O6-C6	-2.90	1.17	1.23
56	w	46	G7M	C2-N1	2.88	1.44	1.37
34	a	1498	UR3	C6-N1	2.88	1.44	1.38
8	A	2251	OMG	C5-C4	-2.88	1.35	1.43
34	a	1207	2MG	C5-C6	2.86	1.53	1.47
34	a	1402	4OC	C6-N1	2.86	1.44	1.38
34	a	966	2MG	C5-C4	-2.86	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2580	PSU	C6-C5	2.84	1.38	1.35
34	a	1519	MA6	C5-C4	-2.84	1.33	1.40
56	w	37	MIA	C5-C4	-2.80	1.33	1.40
8	A	955	PSU	C6-C5	2.79	1.38	1.35
8	A	1915	3TD	C4-N3	2.78	1.46	1.40
8	A	1618	6MZ	C2-N3	2.74	1.36	1.32
34	a	1518	MA6	C5-C4	-2.72	1.33	1.40
56	w	54	5MU	O4-C4	-2.70	1.18	1.23
8	A	2251	OMG	C5-C6	2.59	1.52	1.47
8	A	746	PSU	C6-C5	2.56	1.38	1.35
8	A	2504	PSU	C6-C5	2.54	1.38	1.35
8	A	2604	PSU	C4-C5	-2.51	1.37	1.44
56	w	54	5MU	O2-C2	-2.50	1.18	1.23
34	a	966	2MG	C5-C6	2.50	1.52	1.47
8	A	2030	6MZ	C2-N3	2.48	1.36	1.32
8	A	2251	OMG	O6-C6	-2.47	1.18	1.23
34	a	1498	UR3	O2-C2	-2.47	1.18	1.22
34	a	527	G7M	C5-C6	2.44	1.51	1.45
8	A	2604	PSU	C6-C5	2.43	1.38	1.35
8	A	2552	OMU	C6-N1	2.41	1.43	1.38
56	w	8	4SU	O2-C2	-2.39	1.18	1.23
8	A	2457	PSU	O4'-C1'	-2.38	1.40	1.43
34	a	1498	UR3	O4-C4	-2.38	1.18	1.23
8	A	2580	PSU	O4'-C1'	-2.37	1.40	1.43
8	A	2251	OMG	C2-N1	2.35	1.43	1.37
8	A	2069	G7M	O6-C6	-2.35	1.18	1.23
8	A	2503	2MA	C2-N1	2.34	1.43	1.36
8	A	2580	PSU	C4-C5	-2.34	1.37	1.44
8	A	2069	G7M	C5-C6	2.32	1.51	1.45
34	a	527	G7M	O6-C6	-2.31	1.18	1.23
8	A	955	PSU	C4-C5	-2.29	1.37	1.44
34	a	516	PSU	C6-C5	2.26	1.38	1.35
8	A	2605	PSU	C4-C5	-2.24	1.37	1.44
56	w	46	G7M	O6-C6	-2.24	1.18	1.23
8	A	1835	2MG	C5-C6	2.18	1.51	1.47
8	A	2445	2MG	C4-N3	-2.17	1.32	1.37
8	A	1618	6MZ	C6-N1	-2.15	1.30	1.34
8	A	1917	PSU	C4-C5	-2.12	1.38	1.44
8	A	2030	6MZ	C6-N1	-2.12	1.31	1.34
8	A	2504	PSU	C4-C5	-2.12	1.38	1.44
8	A	2503	2MA	C6-N1	2.12	1.42	1.38
8	A	746	PSU	C4-C5	-2.07	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1911	PSU	C4-C5	-2.07	1.38	1.44
34	a	1498	UR3	C5-C4	2.07	1.49	1.43
8	A	2504	PSU	O4'-C1'	-2.06	1.41	1.43
8	A	2552	OMU	C5-C4	2.06	1.48	1.43
8	A	2457	PSU	C4-C5	-2.03	1.38	1.44
8	A	2457	PSU	C6-C5	2.03	1.37	1.35
8	A	1917	PSU	O4'-C1'	-2.01	1.41	1.43
56	w	8	4SU	C6-N1	2.00	1.42	1.38

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	w	37	MIA	C11-S10-C2	17.08	115.02	102.27
8	A	1939	5MU	C5-C4-N3	12.70	126.15	115.31
56	w	54	5MU	C5-C4-N3	12.05	125.60	115.31
8	A	1939	5MU	C5-C6-N1	-11.25	111.76	123.34
34	a	1518	MA6	N1-C6-N6	-10.20	106.32	117.06
56	w	54	5MU	C5-C6-N1	-9.97	113.09	123.34
34	a	1519	MA6	N1-C6-N6	-9.46	107.10	117.06
56	w	37	MIA	C12-C13-C14	-9.23	109.17	127.14
56	w	8	4SU	C4-N3-C2	-7.30	120.25	127.34
8	A	2030	6MZ	C9-N6-C6	-6.98	116.86	122.87
34	a	1519	MA6	N3-C2-N1	-5.56	119.98	128.68
8	A	1939	5MU	C4-N3-C2	-5.54	120.17	127.35
8	A	2552	OMU	C4-N3-C2	-5.49	119.33	126.58
8	A	2580	PSU	N1-C2-N3	5.47	121.33	115.13
34	a	1518	MA6	N3-C2-N1	-5.42	120.21	128.68
8	A	2030	6MZ	N3-C2-N1	-5.39	120.26	128.68
56	w	8	4SU	C5-C4-N3	5.38	119.67	114.69
8	A	1939	5MU	O4-C4-C5	-5.37	118.67	124.90
8	A	2457	PSU	N1-C2-N3	5.32	121.16	115.13
8	A	2457	PSU	C4-N3-C2	-5.24	118.79	126.34
8	A	746	PSU	C4-N3-C2	-5.11	118.97	126.34
8	A	1939	5MU	N3-C2-N1	5.03	121.56	114.89
8	A	1917	PSU	C4-N3-C2	-5.01	119.12	126.34
8	A	2604	PSU	C4-N3-C2	-4.99	119.14	126.34
8	A	955	PSU	C4-N3-C2	-4.95	119.21	126.34
8	A	1911	PSU	C4-N3-C2	-4.94	119.22	126.34
8	A	1917	PSU	N1-C2-N3	4.90	120.68	115.13
8	A	1618	6MZ	N3-C2-N1	-4.84	121.12	128.68
8	A	955	PSU	N1-C2-N3	4.82	120.59	115.13
8	A	2605	PSU	C4-N3-C2	-4.74	119.50	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	w	54	5MU	C4-N3-C2	-4.72	121.25	127.35
8	A	2604	PSU	N1-C2-N3	4.71	120.46	115.13
56	w	55	PSU	N1-C2-N3	4.69	120.45	115.13
8	A	1911	PSU	N1-C2-N3	4.69	120.44	115.13
8	A	2580	PSU	C4-N3-C2	-4.66	119.62	126.34
8	A	1915	3TD	N1-C2-N3	4.66	119.81	116.14
56	w	54	5MU	O4-C4-C5	-4.65	119.51	124.90
8	A	2552	OMU	N3-C2-N1	4.64	121.05	114.89
56	w	39	PSU	N1-C2-N3	4.59	120.33	115.13
56	w	32	PSU	C4-N3-C2	-4.53	119.81	126.34
56	w	39	PSU	C4-N3-C2	-4.51	119.84	126.34
8	A	2504	PSU	C4-N3-C2	-4.51	119.84	126.34
56	w	37	MIA	C16-C14-C13	-4.49	109.68	122.65
56	w	32	PSU	N1-C2-N3	4.46	120.19	115.13
8	A	746	PSU	N1-C2-N3	4.40	120.11	115.13
8	A	2605	PSU	N1-C2-N3	4.37	120.08	115.13
56	w	54	5MU	N3-C2-N1	4.36	120.68	114.89
56	w	55	PSU	C4-N3-C2	-4.34	120.08	126.34
56	w	37	MIA	C15-C14-C13	-4.27	110.31	122.65
56	w	54	5MU	C5M-C5-C6	-4.21	117.22	122.85
34	a	1498	UR3	C4-N3-C2	-4.18	120.63	124.56
56	w	54	5MU	C5M-C5-C4	4.13	123.32	118.77
8	A	2504	PSU	N1-C2-N3	3.98	119.64	115.13
8	A	1962	5MC	C5-C6-N1	-3.98	119.25	123.34
56	w	8	4SU	C5-C4-S4	-3.95	119.37	124.47
8	A	2030	6MZ	C1'-N9-C4	-3.89	119.81	126.64
56	w	37	MIA	N3-C2-N1	-3.87	119.86	126.98
34	a	1407	5MC	C5-C6-N1	-3.84	119.38	123.34
8	A	1835	2MG	C5-C6-N1	3.84	120.73	113.95
8	A	745	1MG	C5-C6-N1	3.82	119.65	113.90
8	A	747	5MC	C5-C6-N1	-3.81	119.42	123.34
8	A	1939	5MU	O2-C2-N1	-3.76	117.79	122.79
34	a	516	PSU	C4-N3-C2	-3.75	120.93	126.34
34	a	516	PSU	N1-C2-N3	3.73	119.36	115.13
34	a	1516	2MG	C5-C6-N1	3.72	120.53	113.95
34	a	967	5MC	C5-C6-N1	-3.62	119.61	123.34
8	A	2251	OMG	C5-C6-N1	3.61	120.32	113.95
8	A	2580	PSU	C6-N1-C2	-3.59	119.01	122.68
8	A	2503	2MA	C5-C6-N1	3.57	120.18	114.02
8	A	2457	PSU	O2-C2-N1	-3.47	118.97	122.79
8	A	1939	5MU	C5M-C5-C6	-3.46	118.22	122.85
34	a	1498	UR3	C1'-N1-C2	3.44	122.80	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1915	3TD	C4-N3-C2	-3.41	120.91	124.61
56	w	37	MIA	C2-N3-C4	3.39	120.00	115.32
8	A	2445	2MG	C5-C6-N1	3.38	119.92	113.95
34	a	1207	2MG	C5-C6-N1	3.35	119.88	113.95
8	A	2251	OMG	C2-N1-C6	-3.26	119.09	125.10
56	w	8	4SU	N3-C2-N1	3.26	119.22	114.89
34	a	966	2MG	C5-C6-N1	3.19	119.59	113.95
34	a	1498	UR3	C6-N1-C2	-3.17	118.94	121.79
34	a	516	PSU	C6-N1-C2	-3.17	119.44	122.68
8	A	2457	PSU	C6-C5-C4	3.16	120.41	118.20
8	A	2504	PSU	O2-C2-N1	-3.13	119.34	122.79
8	A	2552	OMU	C5-C4-N3	3.04	119.39	114.84
8	A	2445	2MG	O2'-C2'-C1'	-3.03	99.65	110.85
34	a	516	PSU	O2-C2-N1	-3.00	119.48	122.79
56	w	55	PSU	O2-C2-N1	-2.97	119.53	122.79
8	A	747	5MC	CM5-C5-C6	-2.96	118.90	122.85
8	A	2604	PSU	O2-C2-N1	-2.94	119.55	122.79
56	w	46	G7M	C2-N1-C6	-2.90	119.76	125.10
8	A	1939	5MU	C5M-C5-C4	2.89	121.95	118.77
34	a	1407	5MC	CM5-C5-C6	-2.86	119.03	122.85
8	A	2445	2MG	C8-N7-C5	2.85	108.42	102.99
8	A	2503	2MA	C8-N7-C5	2.84	108.41	102.99
8	A	745	1MG	CM1-N1-C6	2.83	121.43	117.55
34	a	527	G7M	C2-N1-C6	-2.80	119.94	125.10
34	a	1498	UR3	O2-C2-N3	-2.79	117.40	121.34
8	A	2552	OMU	O4-C4-C5	-2.77	120.29	125.16
8	A	2580	PSU	C6-C5-C4	2.74	120.12	118.20
8	A	1911	PSU	O2-C2-N1	-2.74	119.77	122.79
8	A	2069	G7M	C2-N1-C6	-2.74	120.06	125.10
8	A	1618	6MZ	C9-N6-C6	-2.73	120.52	122.87
56	w	54	5MU	O4-C4-N3	-2.73	114.89	120.12
34	a	1516	2MG	C8-N7-C5	2.70	108.14	102.99
8	A	745	1MG	C8-N7-C5	2.69	108.12	102.99
8	A	1917	PSU	O2-C2-N1	-2.67	119.86	122.79
8	A	2605	PSU	O2-C2-N1	-2.66	119.86	122.79
8	A	955	PSU	C6-N1-C2	-2.66	119.97	122.68
8	A	1835	2MG	O6-C6-C5	-2.62	119.25	124.37
34	a	1207	2MG	C8-N7-C5	2.61	107.96	102.99
8	A	1939	5MU	O4-C4-N3	-2.58	115.17	120.12
8	A	746	PSU	C6-C5-C4	2.56	119.99	118.20
8	A	2580	PSU	O2-C2-N1	-2.55	119.98	122.79
8	A	1835	2MG	CM2-N2-C2	-2.55	118.24	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	w	32	PSU	O2-C2-N1	-2.55	119.99	122.79
8	A	746	PSU	O2-C2-N1	-2.54	119.99	122.79
8	A	2251	OMG	C8-N7-C5	2.54	107.84	102.99
8	A	2445	2MG	CM2-N2-C2	-2.51	118.32	123.86
8	A	2251	OMG	O6-C6-C5	-2.51	119.47	124.37
8	A	2457	PSU	C6-N1-C2	-2.50	120.13	122.68
8	A	1835	2MG	C8-N7-C5	2.48	107.72	102.99
56	w	55	PSU	C6-N1-C2	-2.45	120.17	122.68
56	w	37	MIA	S10-C2-N1	2.45	124.48	116.01
8	A	2552	OMU	O2-C2-N1	-2.44	119.54	122.79
34	a	1516	2MG	O6-C6-C5	-2.40	119.68	124.37
56	w	39	PSU	C6-N1-C2	-2.40	120.23	122.68
34	a	1516	2MG	CM2-N2-C2	-2.38	118.60	123.86
8	A	955	PSU	O2-C2-N1	-2.38	120.17	122.79
8	A	2457	PSU	O4'-C1'-C2'	2.37	108.48	105.14
8	A	2605	PSU	C6-N1-C2	-2.35	120.28	122.68
8	A	2604	PSU	C6-C5-C4	2.35	119.84	118.20
34	a	966	2MG	C8-N7-C5	2.33	107.43	102.99
8	A	745	1MG	O6-C6-C5	-2.31	120.09	124.19
8	A	2604	PSU	C6-N1-C2	-2.31	120.32	122.68
8	A	1917	PSU	C6-N1-C2	-2.31	120.33	122.68
34	a	966	2MG	O6-C6-C5	-2.29	119.90	124.37
8	A	1911	PSU	C6-N1-C2	-2.29	120.34	122.68
8	A	2445	2MG	O6-C6-N1	-2.29	117.95	120.65
8	A	2580	PSU	O4'-C1'-C2'	2.24	108.31	105.14
34	a	1402	4OC	C6-C5-C4	2.24	119.70	116.96
56	w	8	4SU	C1'-N1-C2	2.22	121.59	117.57
8	A	2445	2MG	C3'-C2'-C1'	2.19	104.27	100.98
56	w	37	MIA	C12-N6-C6	-2.18	119.32	122.55
56	w	54	5MU	O2-C2-N1	-2.16	119.92	122.79
8	A	1939	5MU	C6-C5-C4	2.14	119.82	118.03
34	a	1207	2MG	O6-C6-C5	-2.13	120.22	124.37
8	A	1917	PSU	C6-C5-C4	2.10	119.67	118.20
8	A	2504	PSU	C6-N1-C2	-2.07	120.56	122.68
56	w	32	PSU	C6-N1-C2	-2.06	120.57	122.68
8	A	2503	2MA	CM2-C2-N1	2.04	120.77	116.23
34	a	516	PSU	O4'-C1'-C2'	2.04	108.02	105.14
34	a	1402	4OC	CM4-N4-C4	-2.04	118.47	122.45
8	A	1962	5MC	CM5-C5-C6	-2.01	120.17	122.85

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	746	PSU	C2'-C1'-C5-C4
8	A	746	PSU	C2'-C1'-C5-C6
8	A	746	PSU	O4'-C1'-C5-C6
8	A	955	PSU	C2'-C1'-C5-C4
8	A	1618	6MZ	C5-C6-N6-C9
8	A	1618	6MZ	N1-C6-N6-C9
8	A	1915	3TD	O4'-C1'-C5-C4
8	A	1915	3TD	O4'-C1'-C5-C6
8	A	2251	OMG	C1'-C2'-O2'-CM2
8	A	2445	2MG	C3'-C4'-C5'-O5'
8	A	2552	OMU	C1'-C2'-O2'-CM2
34	a	516	PSU	C2'-C1'-C5-C4
34	a	516	PSU	C2'-C1'-C5-C6
34	a	966	2MG	C3'-C4'-C5'-O5'
34	a	967	5MC	O4'-C4'-C5'-O5'
34	a	1498	UR3	O4'-C4'-C5'-O5'
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C2
34	a	1518	MA6	C5-C6-N6-C10
56	w	32	PSU	C2'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C4
56	w	32	PSU	O4'-C1'-C5-C6
56	w	37	MIA	C5-C6-N6-C12
56	w	37	MIA	N1-C6-N6-C12
56	w	37	MIA	N1-C2-S10-C11
56	w	37	MIA	N3-C2-S10-C11
56	w	37	MIA	C12-C13-C14-C15
56	w	37	MIA	C12-C13-C14-C16
56	w	39	PSU	C2'-C1'-C5-C4
56	w	39	PSU	O4'-C1'-C5-C4
56	w	39	PSU	O4'-C1'-C5-C6
56	w	46	G7M	O4'-C4'-C5'-O5'
56	w	46	G7M	C3'-C4'-C5'-O5'
8	A	2552	OMU	O4'-C1'-N1-C2
8	A	2030	6MZ	O4'-C4'-C5'-O5'
8	A	2503	2MA	O4'-C4'-C5'-O5'
34	a	967	5MC	C3'-C4'-C5'-O5'
34	a	1498	UR3	C3'-C4'-C5'-O5'
56	w	37	MIA	O4'-C4'-C5'-O5'
34	a	966	2MG	O4'-C4'-C5'-O5'
34	a	1207	2MG	O4'-C4'-C5'-O5'
34	a	1207	2MG	C3'-C4'-C5'-O5'
8	A	2445	2MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
56	w	32	PSU	C3'-C4'-C5'-O5'
56	w	37	MIA	C3'-C4'-C5'-O5'
8	A	1835	2MG	O4'-C4'-C5'-O5'
8	A	2504	PSU	O4'-C4'-C5'-O5'
8	A	2552	OMU	O4'-C4'-C5'-O5'
8	A	2552	OMU	O4'-C1'-N1-C6
34	a	1518	MA6	C5-C6-N6-C9
8	A	1835	2MG	C3'-C4'-C5'-O5'
8	A	2503	2MA	C3'-C4'-C5'-O5'
8	A	2504	PSU	C3'-C4'-C5'-O5'
8	A	2552	OMU	C3'-C4'-C5'-O5'
34	a	967	5MC	C4'-C5'-O5'-P
8	A	747	5MC	C3'-C4'-C5'-O5'
56	w	32	PSU	O4'-C4'-C5'-O5'
8	A	2030	6MZ	C3'-C4'-C5'-O5'
8	A	1915	3TD	C3'-C4'-C5'-O5'
8	A	747	5MC	C4'-C5'-O5'-P
34	a	1498	UR3	C2'-C1'-N1-C6
8	A	2498	OMC	C4'-C5'-O5'-P
34	a	1207	2MG	C4'-C5'-O5'-P
8	A	746	PSU	O4'-C1'-C5-C4
8	A	955	PSU	O4'-C1'-C5-C4
8	A	1911	PSU	O4'-C1'-C5-C4
8	A	2605	PSU	O4'-C1'-C5-C4
34	a	1518	MA6	N1-C6-N6-C10
8	A	2498	OMC	O4'-C4'-C5'-O5'
34	a	527	G7M	C4'-C5'-O5'-P
8	A	747	5MC	O4'-C4'-C5'-O5'
8	A	955	PSU	O4'-C1'-C5-C6
8	A	2605	PSU	O4'-C1'-C5-C6
56	w	55	PSU	O4'-C4'-C5'-O5'
8	A	2069	G7M	O4'-C4'-C5'-O5'
34	a	1498	UR3	C2'-C1'-N1-C2
56	w	46	G7M	C4'-C5'-O5'-P
34	a	967	5MC	O4'-C1'-N1-C6

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 257 ligands modelled in this entry, 257 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 (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

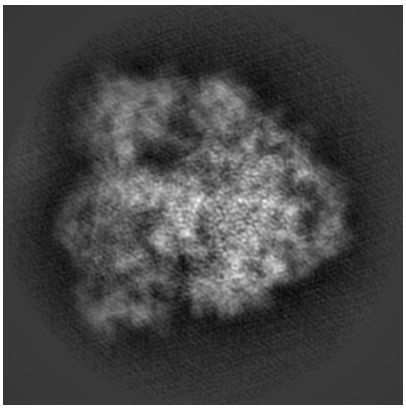
5 Map visualisation

This section contains visualisations of the EMDB entry EMD-10907. These allow visual inspection of the internal detail of the map and identification of artifacts.

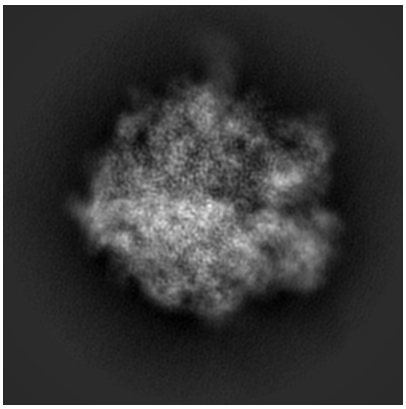
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections

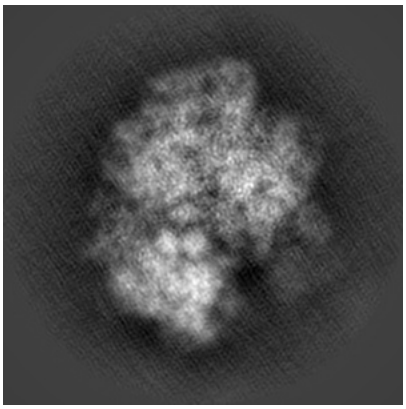
5.1.1 Primary map



X

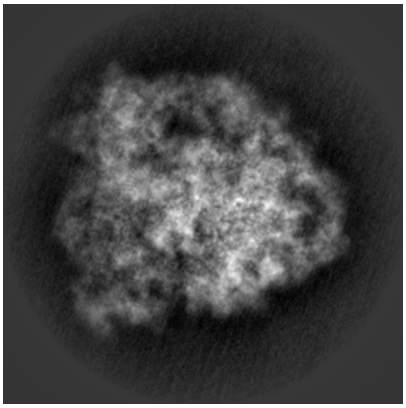


Y

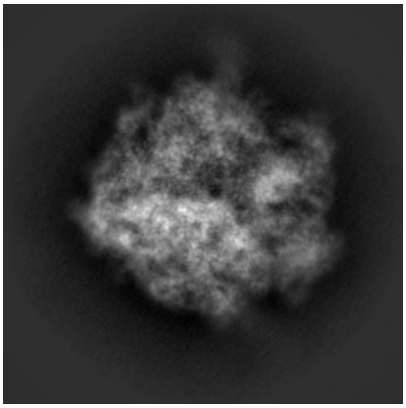


Z

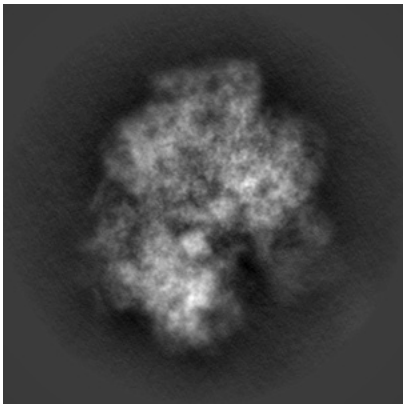
5.1.2 Raw map



X



Y

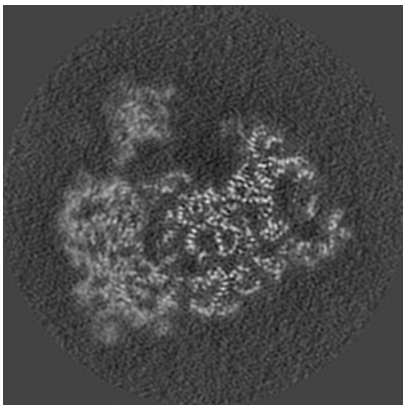


Z

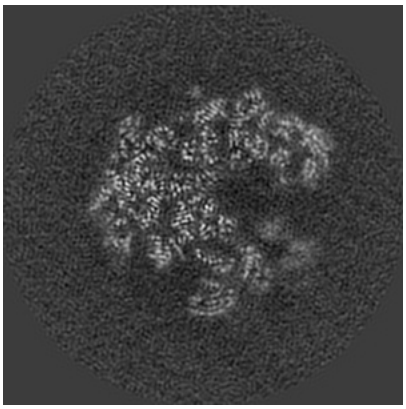
The images above show the map projected in three orthogonal directions.

5.2 Central slices (i)

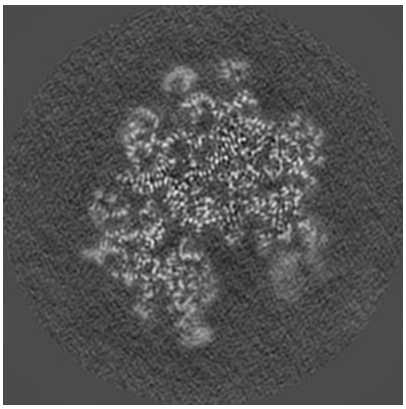
5.2.1 Primary map



X Index: 144

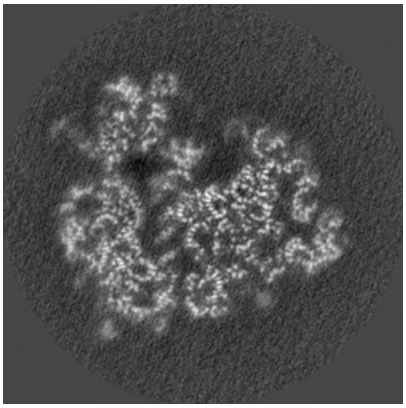


Y Index: 144

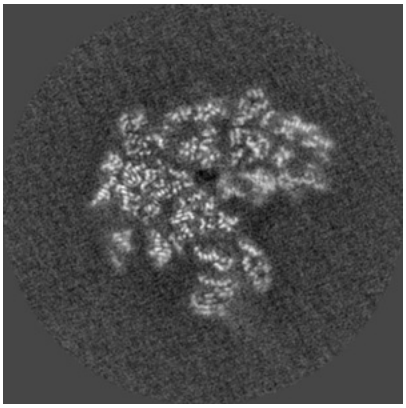


Z Index: 144

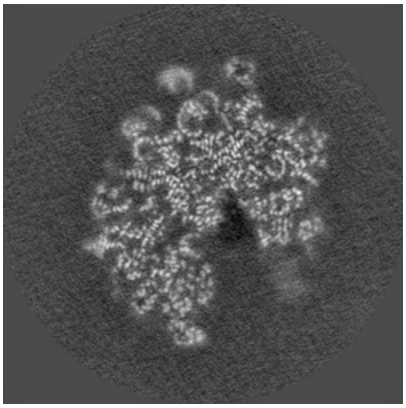
5.2.2 Raw map



X Index: 144



Y Index: 144

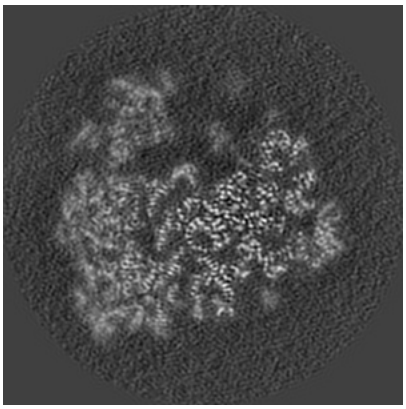


Z Index: 144

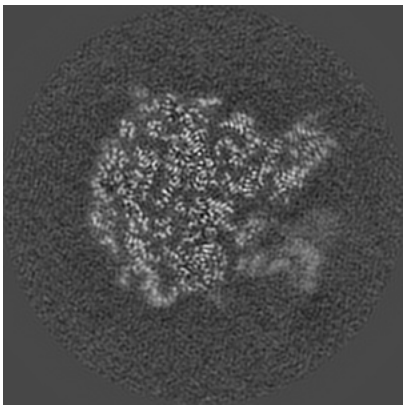
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices (i)

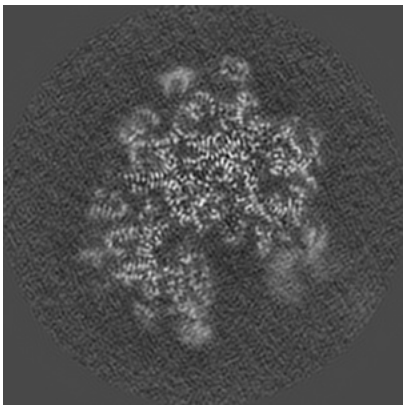
5.3.1 Primary map



X Index: 138

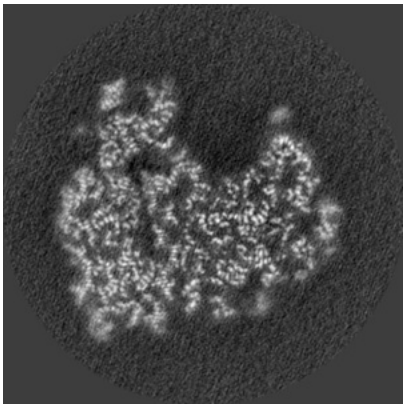


Y Index: 165

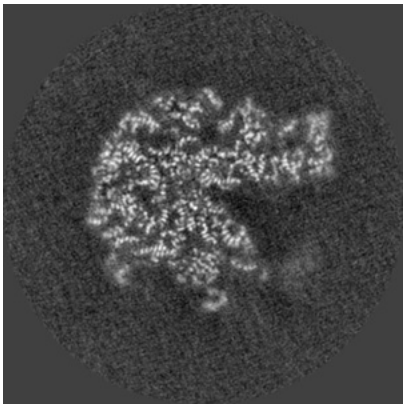


Z Index: 146

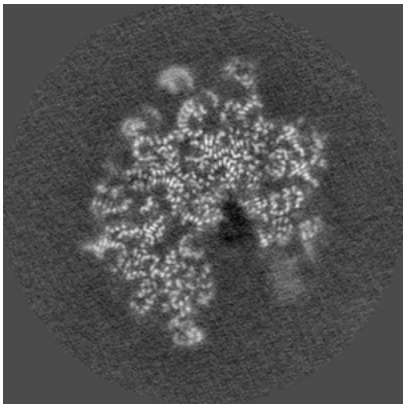
5.3.2 Raw map



X Index: 136



Y Index: 157

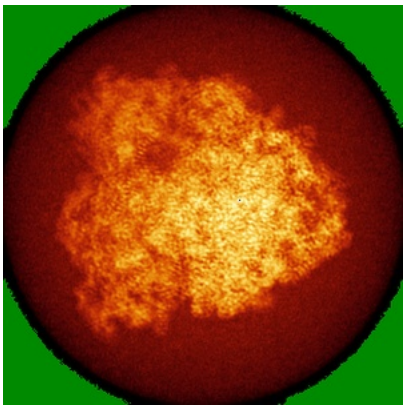


Z Index: 145

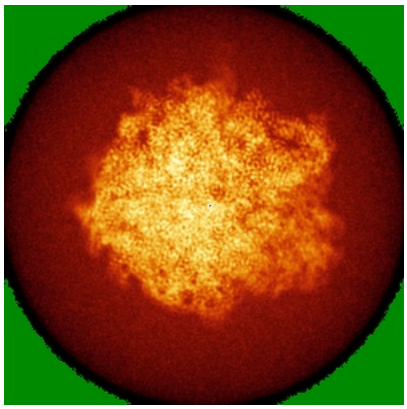
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) (i)

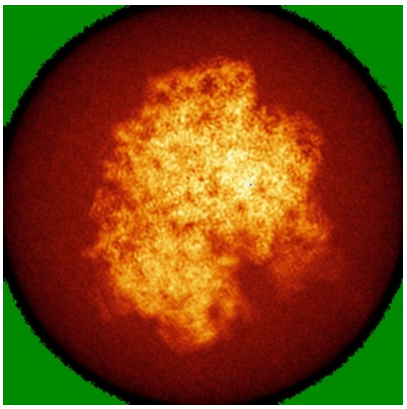
5.4.1 Primary map



X

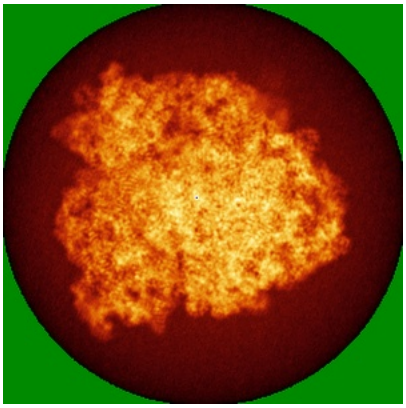


Y

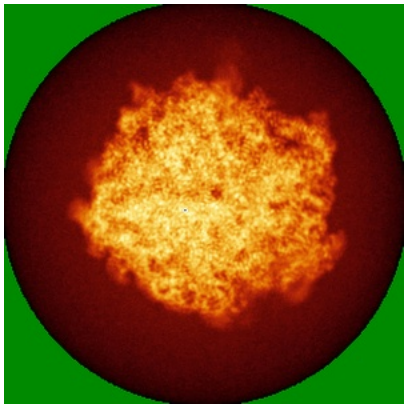


Z

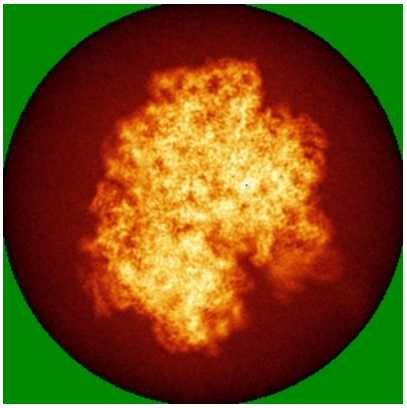
5.4.2 Raw map



X



Y

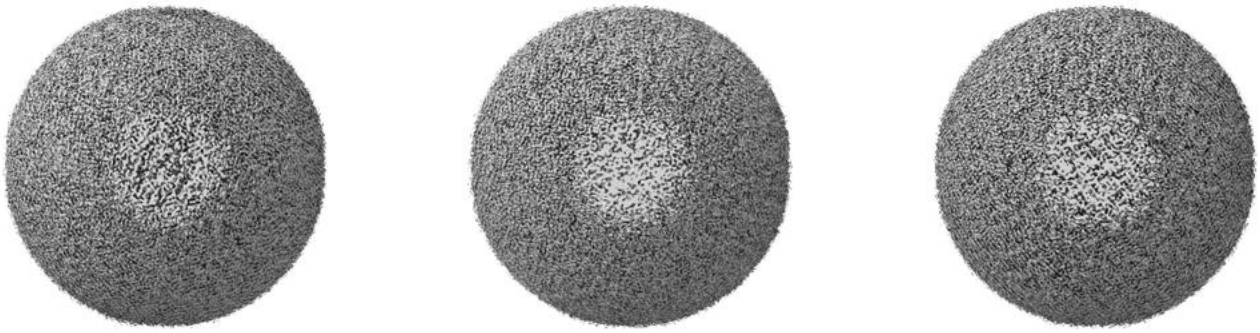


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views (i)

5.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

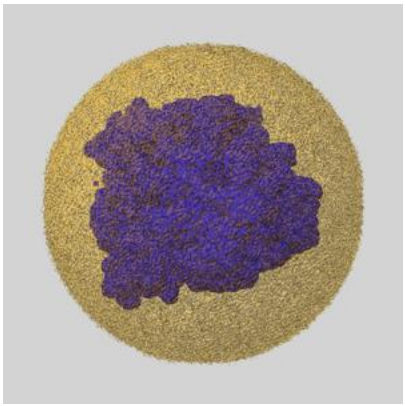
5.6 Mask visualisation (i)

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

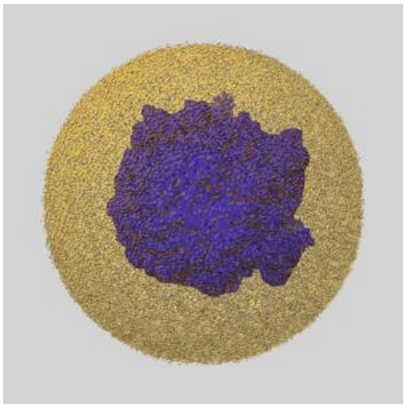
A mask typically either:

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

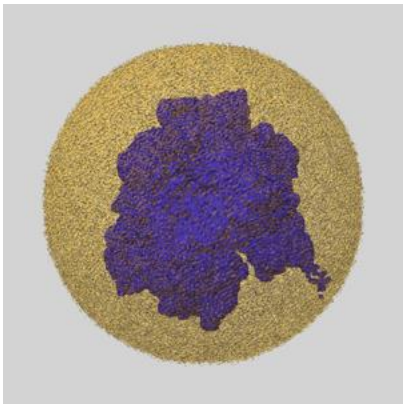
5.6.1 emd_10907_msk_1.map (i)



X



Y

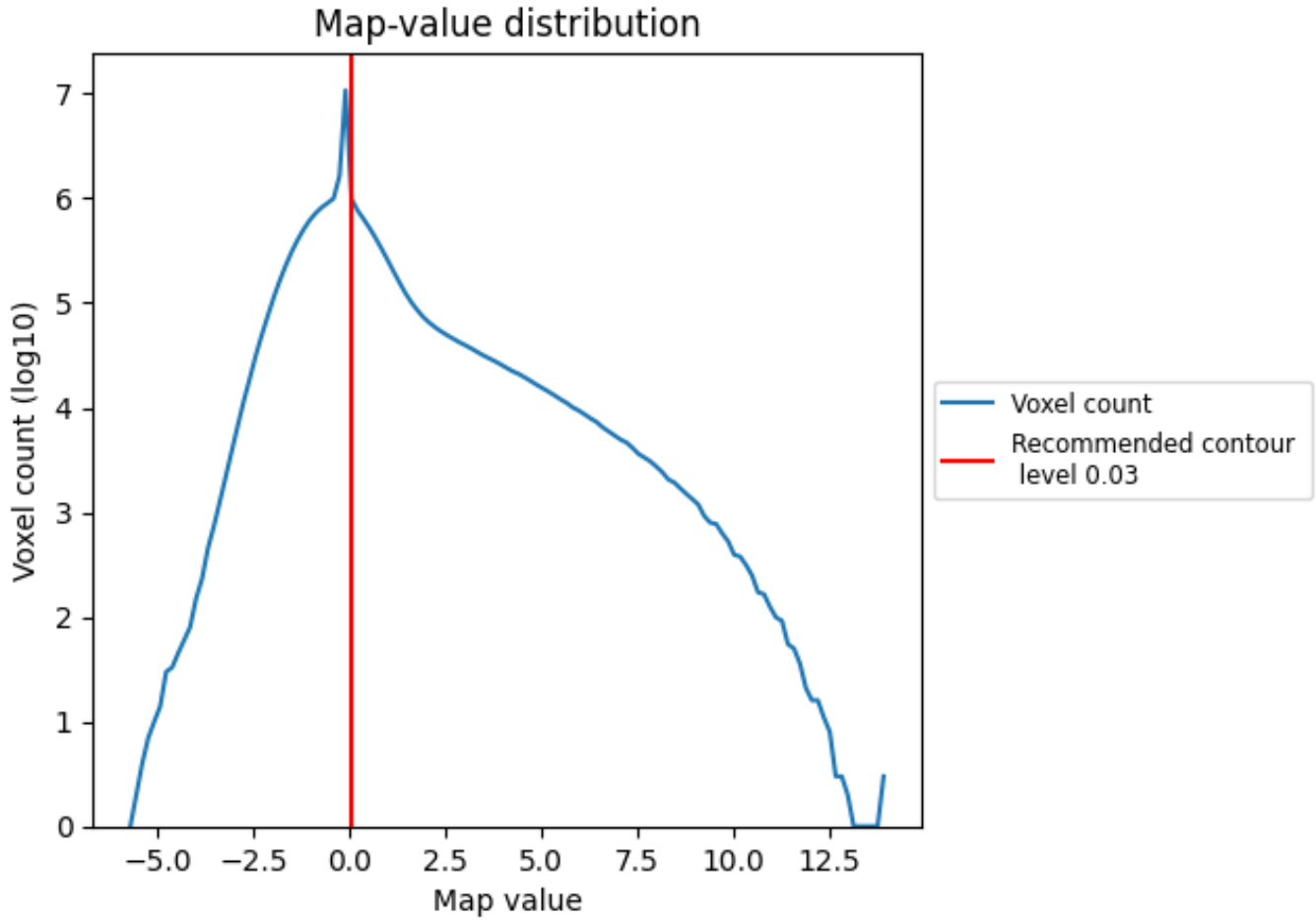


Z

6 Map analysis

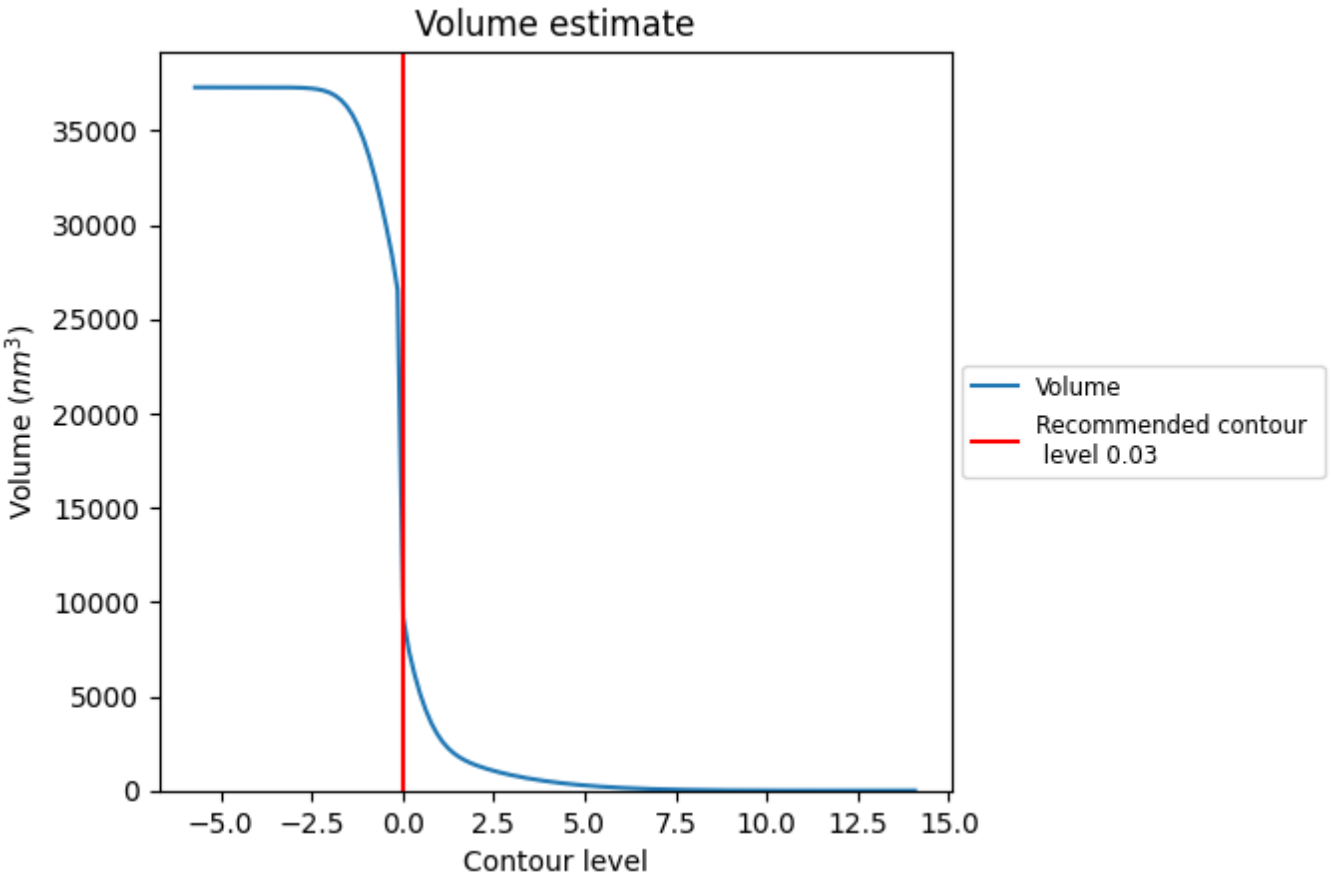
This section contains the results of statistical analysis of the map.

6.1 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.

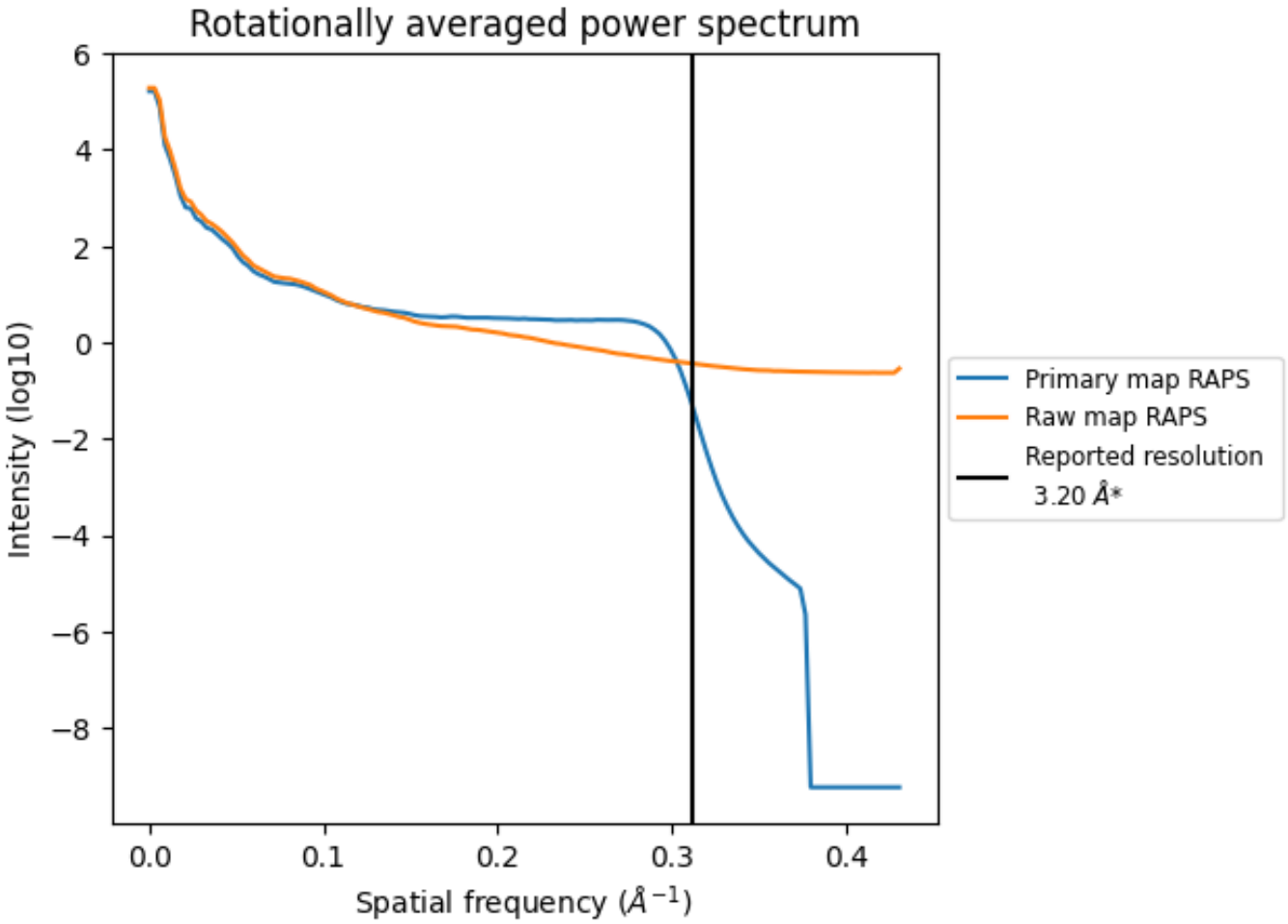
6.2 Volume estimate



The volume at the recommended contour level is 9022 nm^3; this corresponds to an approximate mass of 8149 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 (i)

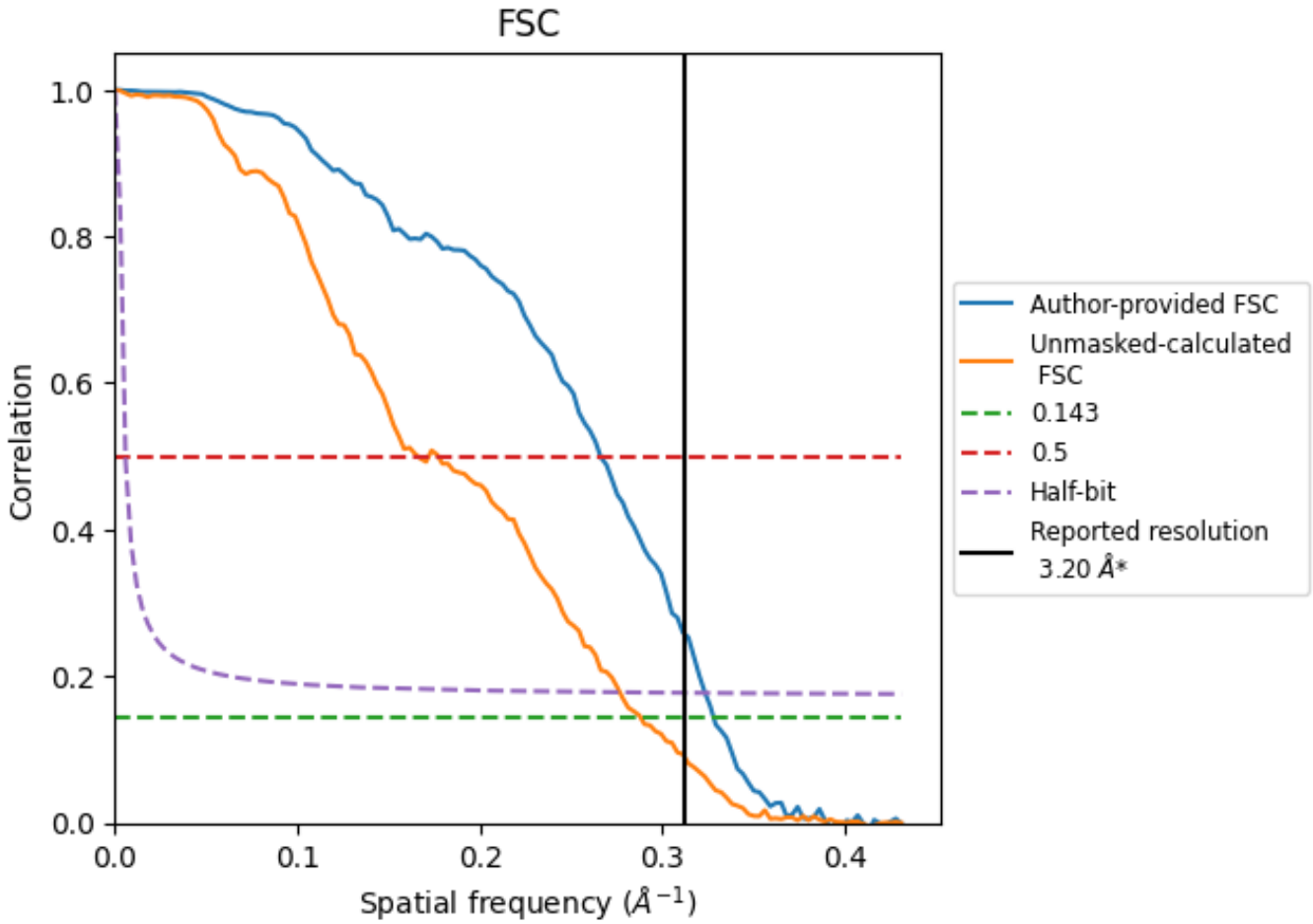


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

7 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.

7.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

7.2 Resolution estimates (i)

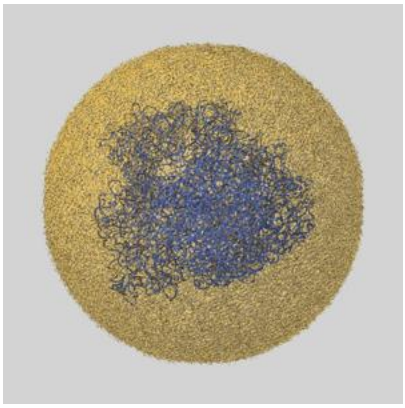
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.05	3.76	3.09
Unmasked-calculated*	3.47	6.02	3.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

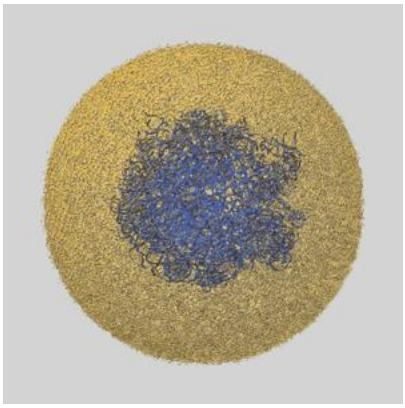
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10907 and PDB model 6YST. Per-residue inclusion information can be found in section ?? on page ??.

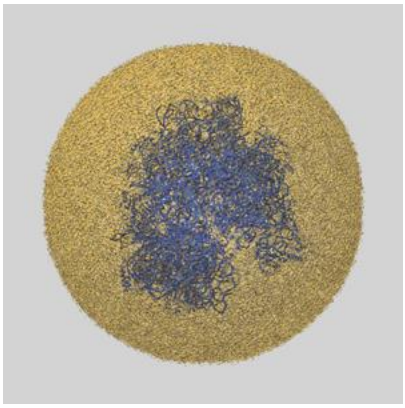
8.1 Map-model overlay



X



Y



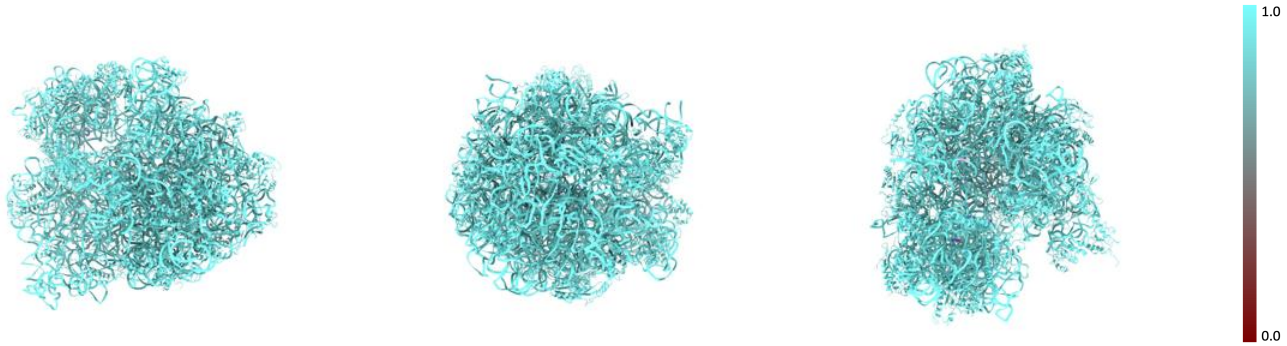
Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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 Q-score mapped to coordinate model (i)

This section was not generated.

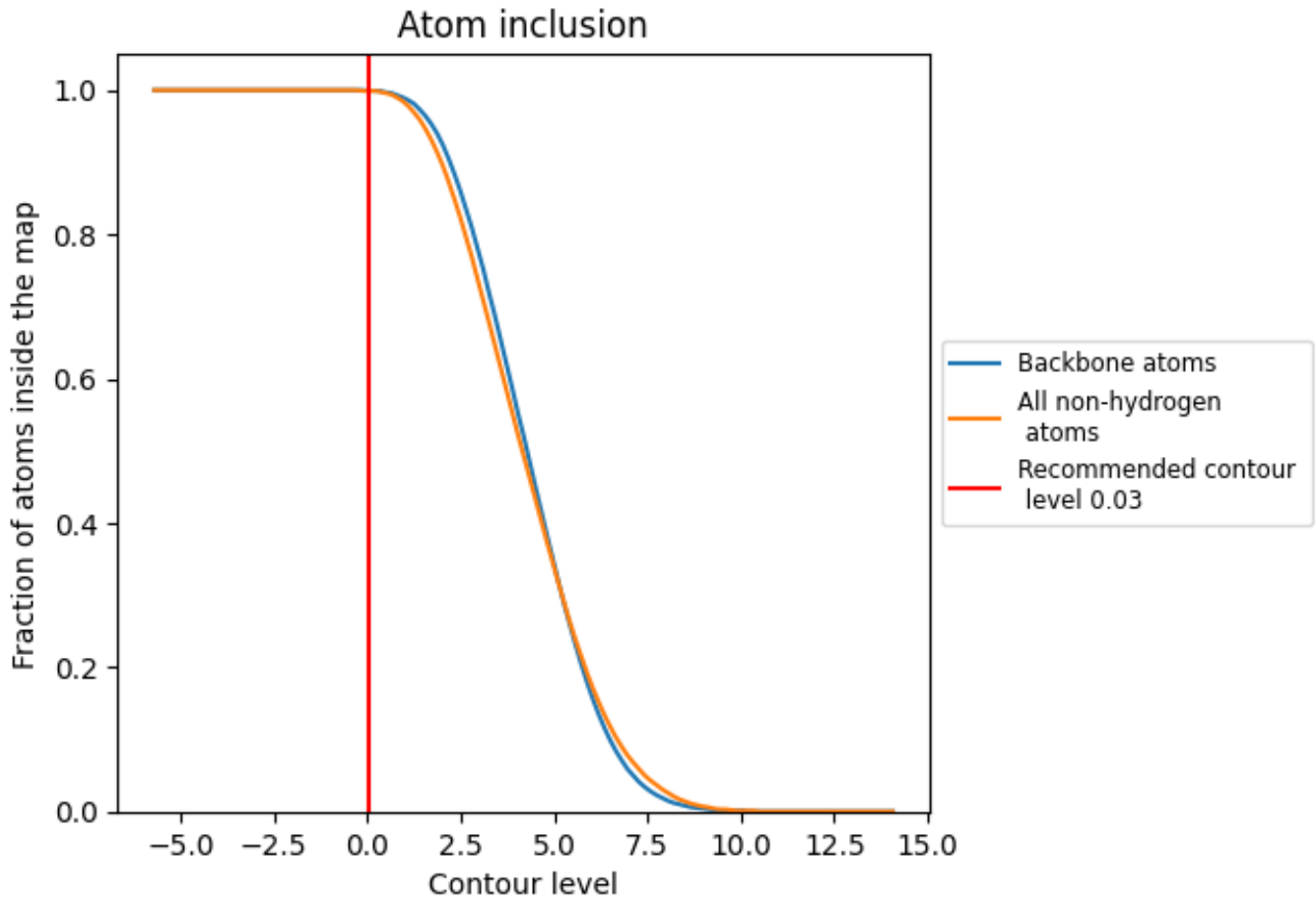
8.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

8.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.9990
0	1.0000
1	0.9980
2	0.9920
3	0.9980
4	1.0000
5	0.9990
6	0.9980
A	1.0000
B	1.0000
C	0.9990
D	0.9990
E	1.0000
F	1.0000
G	1.0000
H	0.9930
I	0.9700
J	1.0000
K	0.9980
L	1.0000
M	0.9990
N	0.9990
O	1.0000
P	1.0000
Q	0.9990
R	1.0000
S	0.9950
T	0.9990
U	1.0000
V	1.0000
W	0.9980
X	1.0000
Y	1.0000
Z	1.0000
a	1.0000

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Chain	Atom inclusion
b	0.9930
c	0.9990
d	0.9990
e	0.9990
f	1.0000
g	0.9970
h	1.0000
i	1.0000
j	0.9990
k	0.9990
l	0.9990
m	1.0000
n	1.0000
o	0.9990
p	1.0000
q	1.0000
r	0.9980
s	1.0000
t	1.0000
u	1.0000
v	1.0000
w	0.9930
x	1.0000
y	0.9980