



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 09:04 PM UTC

PDB ID : 6GQB / pdb_00006gqb
EMDB ID : EMD-0048
Title : Cryo-EM reconstruction of yeast 80S ribosome in complex with mRNA, tRNA and eEF2 (GDP+AlF₄/sordarin)
Authors : Pellegrino, S.; Yusupov, M.; Yusupova, G.; Hashem, Y.
Deposited on : 2018-06-07
Resolution : 3.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

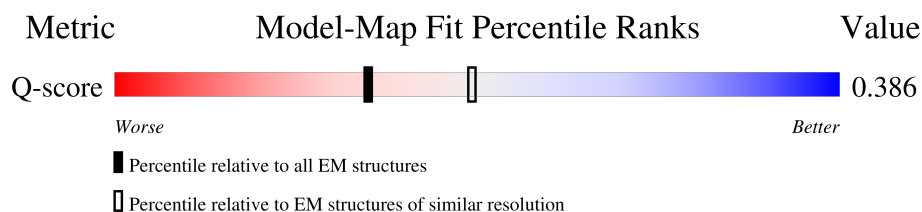
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	8855 (3.40 - 4.40)

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

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 212143 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called *Saccharomyces cerevisiae* S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3223	Total	C	N	O	P	0	0
			68931	30790	12416	22502	3223		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 4 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P0	189	Total	C	N	O	S	0	0
			1473	942	257	270	4		

- Molecule 5 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P2	94	Total	C	N	O	S	0	0
			723	448	138	135	2		

- Molecule 6 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 8 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 10 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 11 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 12 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 13 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 14 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	211	Total	C	N	O	S	0	0
			1705	1083	322	294	6		

- Molecule 15 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 16 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	193	Total	C	N	O	S	0	0
			1543	962	315	266			

- Molecule 17 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 18 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 19 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 20 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	183	Total	C	N	O	S	0	0
			1420	882	281	257			

- Molecule 21 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 22 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	188	Total	C	N	O		0	0
			1521	935	326	260			

- Molecule 23 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 24 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 25 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	100	Total	C	N	O		0	0
			796	516	131	149			

- Molecule 26 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 27 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	64	Total	C	N	O	S	0	0
			528	340	103	84	1		

- Molecule 28 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 29 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 30 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 31 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	58	Total	C	N	O		0	0
			462	289	100	73			

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 34 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 36 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 37 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 38 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 39 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 40 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 41 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 42 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 43 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 44 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 45 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 46 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	2	1776	Total	C	N	O	P	0	0
			37845	16918	6702	12449	1776		

- Molecule 48 is a protein called 40S ribosomal protein S0-A.

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

- Molecule 49 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 50 is a protein called 40S ribosomal protein S2.

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

- Molecule 51 is a protein called 40S ribosomal protein S3.

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

- Molecule 52 is a protein called 40S ribosomal protein S4-A.

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

- Molecule 53 is a protein called 40S ribosomal protein S5.

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

- Molecule 54 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	223	Total	C	N	O	S	0	0
			1790	1123	346	318	3		

- Molecule 55 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	x	184	Total	C	N	O	0	0
			1481	951	265	265		

- Molecule 56 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 57 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 58 is a protein called 40S ribosomal protein S10-A.

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

- Molecule 59 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AB	153	Total	C	N	O	S	0	0
			1220	780	231	206	3		

- Molecule 60 is a protein called 40S ribosomal protein S12.

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

- Molecule 61 is a protein called 40S ribosomal protein S13.

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

- Molecule 62 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AE	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 63 is a protein called 40S ribosomal protein S15.

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

- Molecule 64 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AG	141	Total	C	N	O	S	0	0
			1105	708	203	194			

- Molecule 65 is a protein called 40S ribosomal protein S17-B.

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

- Molecule 66 is a protein called 40S ribosomal protein S18-A.

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

- Molecule 67 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 68 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AK	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 69 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 70 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 71 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 72 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 73 is a protein called 40S ribosomal protein S25-A.

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

- Molecule 74 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AQ	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 75 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 76 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 77 is a protein called 40S ribosomal protein S29-A.

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

- Molecule 78 is a protein called 40S ribosomal protein S30-A.

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

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

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

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AW	37	Total	C	N	O	S	0	0
			287	177	57	49	4		

- Molecule 81 is a RNA chain called Transfer RNA - Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AX	76	Total	C	N	O	P	0	0
			1626	725	293	532	76		

- Molecule 82 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	AY	7	Total	C	N	O	P	0	0
			144	65	21	51	7		

- Molecule 83 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	BA	204	Total	C	N	O	S	0	0
			1609	1031	279	290	9		

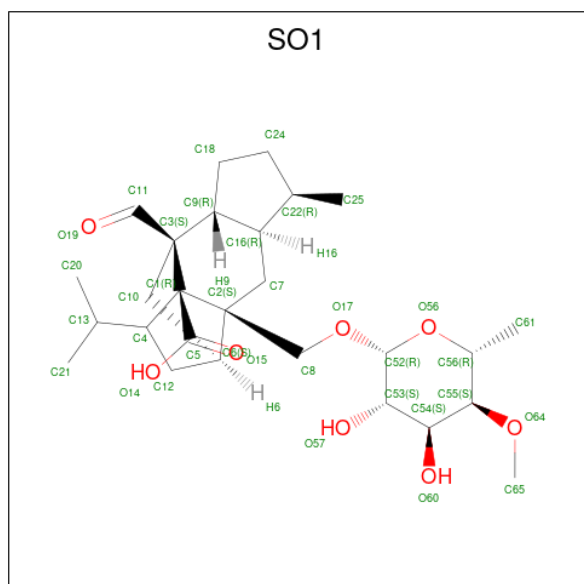
- Molecule 84 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	AZ	840	Total	C	N	O	S	0	0
			6551	4161	1124	1237	29		

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

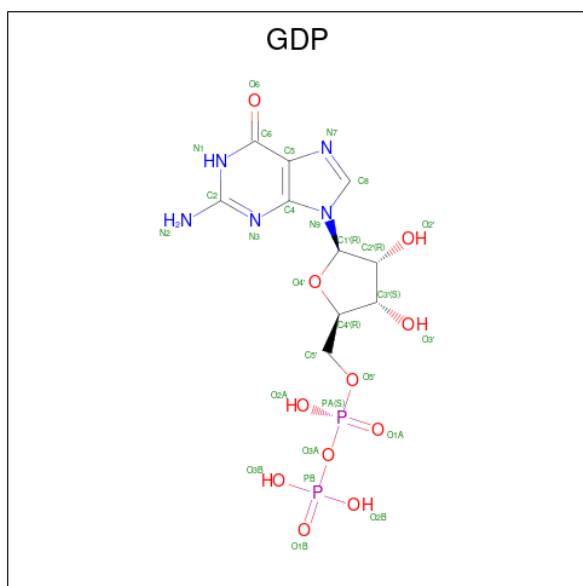
Mol	Chain	Residues	Atoms		AltConf
85	j	1	Total	Zn	0
			1	1	
85	m	1	Total	Zn	0
			1	1	
85	o	1	Total	Zn	0
			1	1	
85	p	1	Total	Zn	0
			1	1	
85	AQ	1	Total	Zn	0
			1	1	
85	AR	1	Total	Zn	0
			1	1	
85	AT	1	Total	Zn	0
			1	1	
85	AW	1	Total	Zn	0
			1	1	

- Molecule 86 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.BETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (CCD ID: SO1) (formula: C₂₇H₄₂O₈).



Mol	Chain	Residues	Atoms			AltConf
86	AZ	1	Total	C	O	0
			35	27	8	

- Molecule 87 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
88	AZ	1	5	1	4	0

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

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77200	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.358	Depositor
Minimum map value	-0.193	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
84	DDE	AZ	699	84	18,20,21	2.08	5 (27%)	17,28,30	1.76	4 (23%)

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
84	DDE	AZ	699	84	-	6/20/21/23	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	AZ	699	DDE	CBI-NAD	6.32	1.47	1.32
84	AZ	699	DDE	CG-ND1	-3.02	1.32	1.38
84	AZ	699	DDE	OAG-CBI	-2.73	1.18	1.23
84	AZ	699	DDE	CAT-CE1	2.59	1.54	1.49
84	AZ	699	DDE	CBW-NCB	-2.20	1.49	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	AZ	699	DDE	OAG-CBI-NAD	-4.26	115.52	123.04
84	AZ	699	DDE	CAU-CBW-CBI	-2.93	105.48	111.22
84	AZ	699	DDE	CAC-NCB-CAB	2.44	117.28	107.99
84	AZ	699	DDE	CA-CB-CG	-2.13	108.52	113.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	AZ	699	DDE	OAG-CBI-CBW-NCB
84	AZ	699	DDE	CAT-CAU-CBW-CBI
84	AZ	699	DDE	CAT-CAU-CBW-NCB
84	AZ	699	DDE	CA-CB-CG-ND1
84	AZ	699	DDE	CE1-CAT-CAU-CBW
84	AZ	699	DDE	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
86	SO1	AZ	901	-	34,39,39	0.14	0	38,64,64	0.88	2 (5%)
88	ALF	AZ	903	-	4,4,4	1.44	0	-		
87	GDP	AZ	902	-	29,30,30	3.39	13 (44%)	45,47,47	1.97	11 (24%)

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
86	SO1	AZ	901	-	-	15/21/104/104	0/7/5/5
87	GDP	AZ	902	-	-	0/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	AZ	902	GDP	C3'-C4'	-7.89	1.33	1.53
87	AZ	902	GDP	O4'-C4'	6.99	1.60	1.45
87	AZ	902	GDP	C4-N3	6.94	1.50	1.34
87	AZ	902	GDP	PA-O3A	5.93	1.65	1.59
87	AZ	902	GDP	C2-N2	5.78	1.47	1.34
87	AZ	902	GDP	C2-N3	5.44	1.46	1.33
87	AZ	902	GDP	O4'-C1'	-4.16	1.32	1.42
87	AZ	902	GDP	C6-N1	3.09	1.44	1.38
87	AZ	902	GDP	C2-N1	2.98	1.44	1.37
87	AZ	902	GDP	C5-C6	2.85	1.55	1.44
87	AZ	902	GDP	C5-N7	-2.44	1.34	1.39
87	AZ	902	GDP	PA-O5'	2.43	1.68	1.59
87	AZ	902	GDP	O2'-C2'	-2.42	1.37	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	AZ	902	GDP	C1'-N9-C4	-5.11	111.38	126.49
87	AZ	902	GDP	C2-N3-C4	4.89	120.71	112.30
87	AZ	902	GDP	C5-C4-N3	-4.83	120.70	128.39
87	AZ	902	GDP	C1'-N9-C8	4.41	139.25	126.73
86	AZ	901	SO1	C18-C9-C16	-4.17	98.02	103.72
87	AZ	902	GDP	N9-C8-N7	-3.61	106.71	113.40
87	AZ	902	GDP	N9-C4-N3	3.01	131.97	125.95
87	AZ	902	GDP	C2-N1-C6	-2.80	120.03	125.11
87	AZ	902	GDP	C5-C6-N1	2.57	119.81	113.25
87	AZ	902	GDP	C8-N7-C5	2.45	108.63	104.26
87	AZ	902	GDP	O6-C6-C5	-2.29	120.49	126.53
86	AZ	901	SO1	C7-C2-C6	2.28	116.42	112.05
87	AZ	902	GDP	N1-C2-N3	-2.22	119.26	123.32

There are no chirality outliers.

All (15) torsion outliers are listed below:

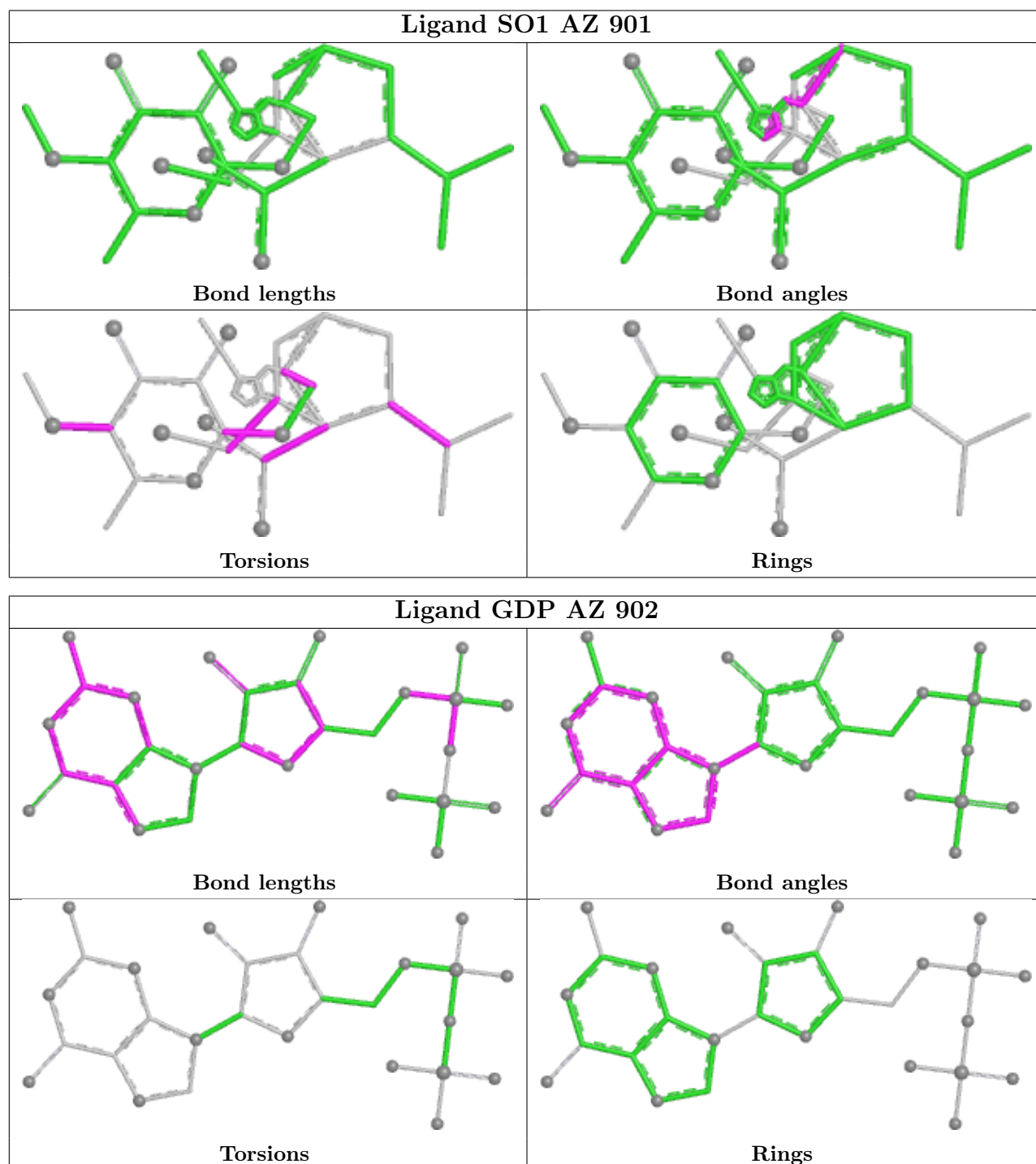
Mol	Chain	Res	Type	Atoms
86	AZ	901	SO1	C2-C1-C5-O14
86	AZ	901	SO1	C2-C1-C5-O15
86	AZ	901	SO1	O19-C11-C3-C1
86	AZ	901	SO1	C56-C55-O64-C65
86	AZ	901	SO1	C21-C13-C4-C12
86	AZ	901	SO1	O56-C52-O17-C8
86	AZ	901	SO1	C20-C13-C4-C12
86	AZ	901	SO1	C7-C2-C8-O17
86	AZ	901	SO1	C1-C2-C8-O17
86	AZ	901	SO1	C20-C13-C4-C1
86	AZ	901	SO1	C21-C13-C4-C1
86	AZ	901	SO1	C4-C1-C5-O14
86	AZ	901	SO1	C54-C55-O64-C65
86	AZ	901	SO1	O19-C11-C3-C10
86	AZ	901	SO1	C6-C2-C8-O17

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

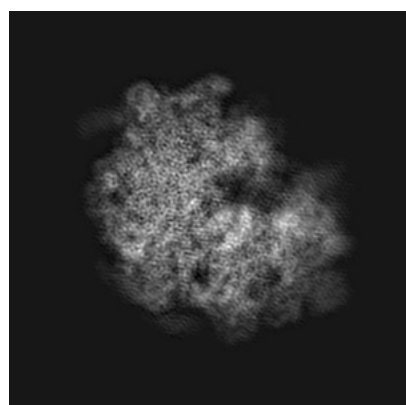
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0048. These allow visual inspection of the internal detail of the map and identification of artifacts.

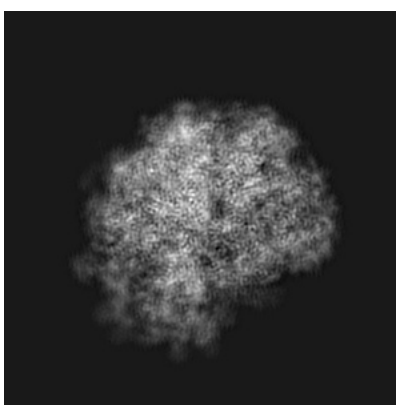
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

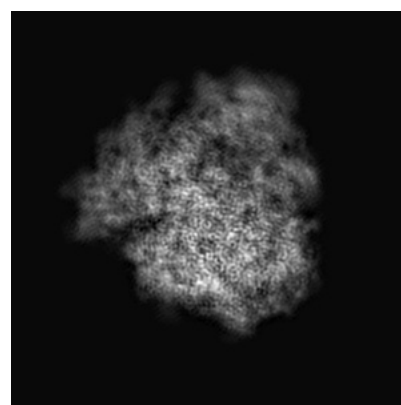
5.1.1 Primary map



X



Y

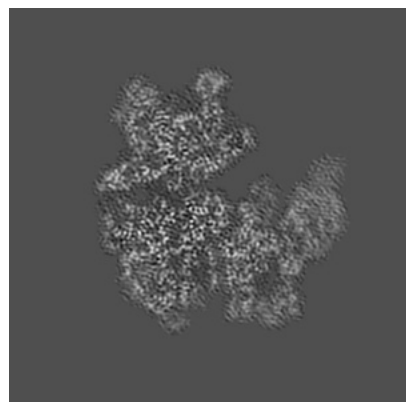


Z

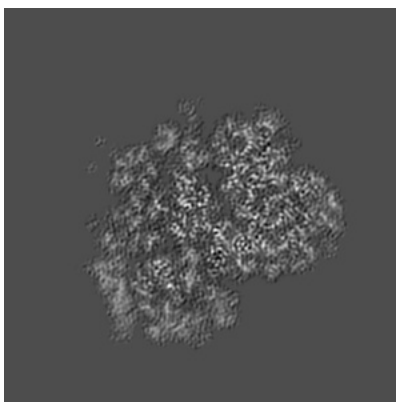
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

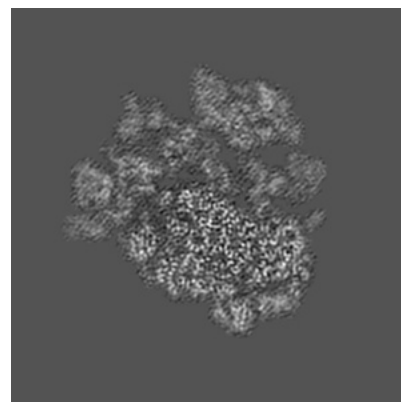
5.2.1 Primary map



X Index: 180



Y Index: 180

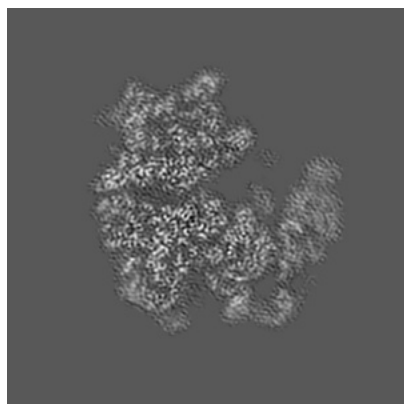


Z Index: 180

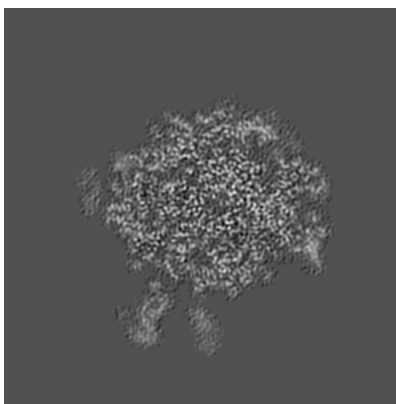
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

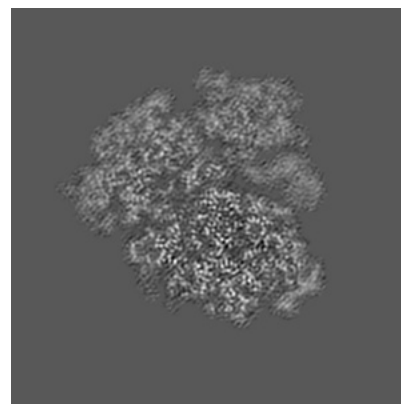
5.3.1 Primary map



X Index: 184



Y Index: 157

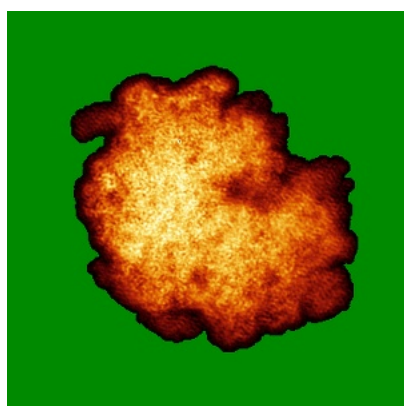


Z Index: 166

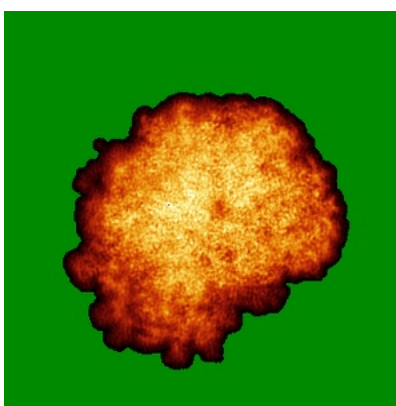
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) [i](#)

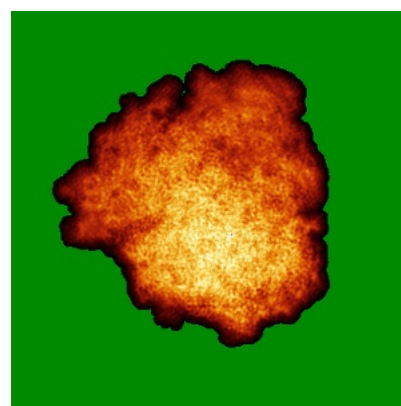
5.4.1 Primary map



X



Y



Z

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

This section was not generated.

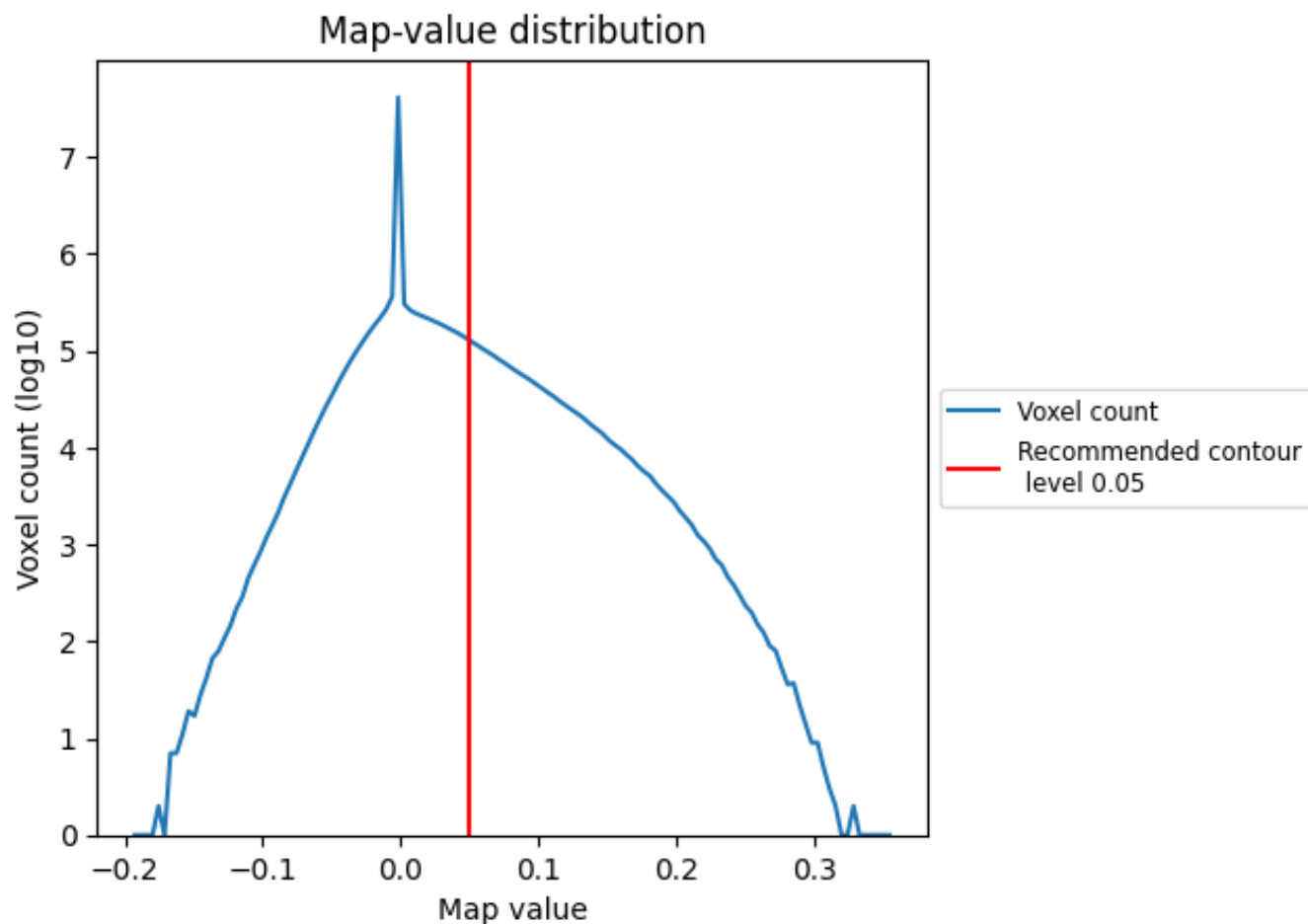
5.6 Mask visualisation

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

6 Map analysis [i](#)

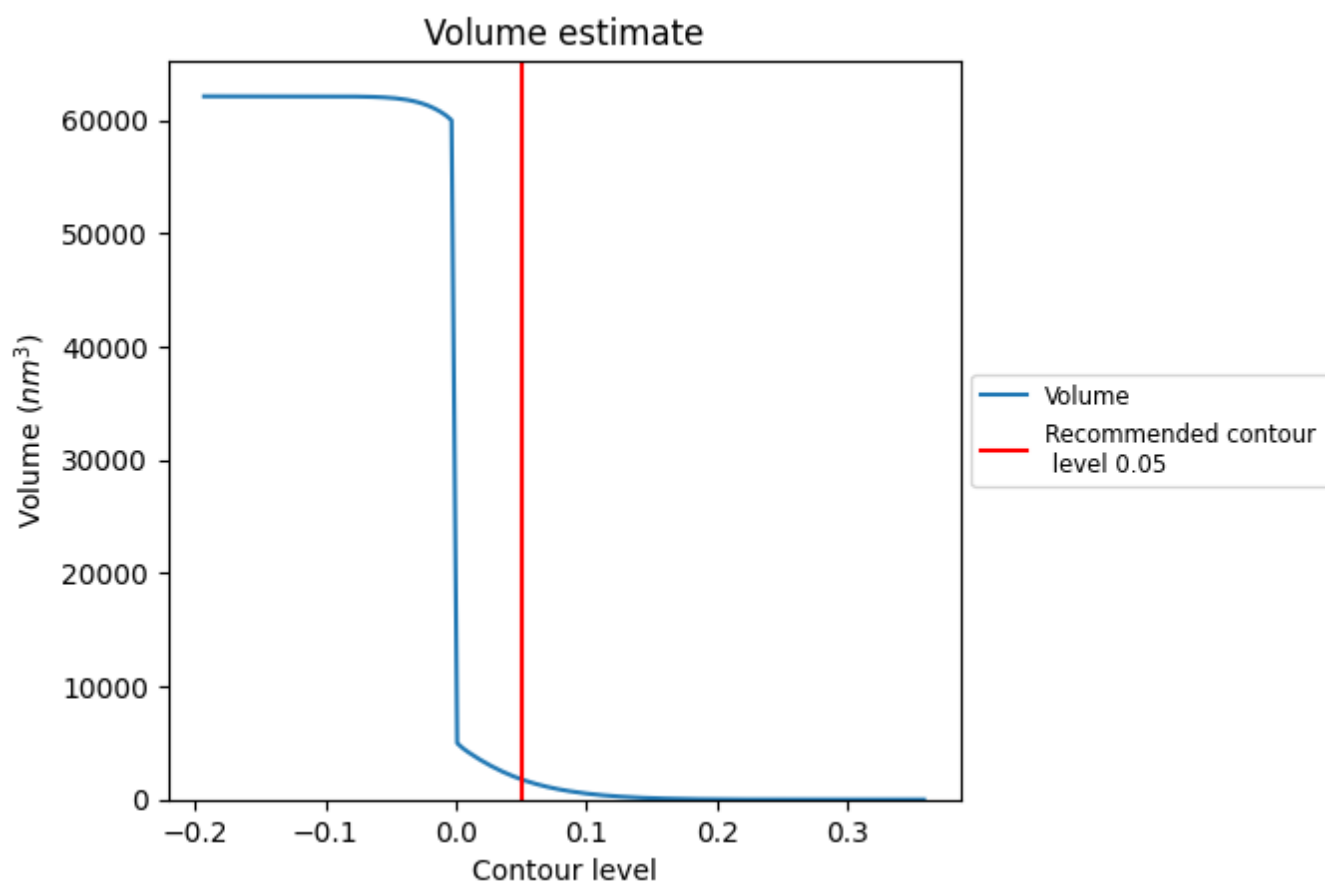
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

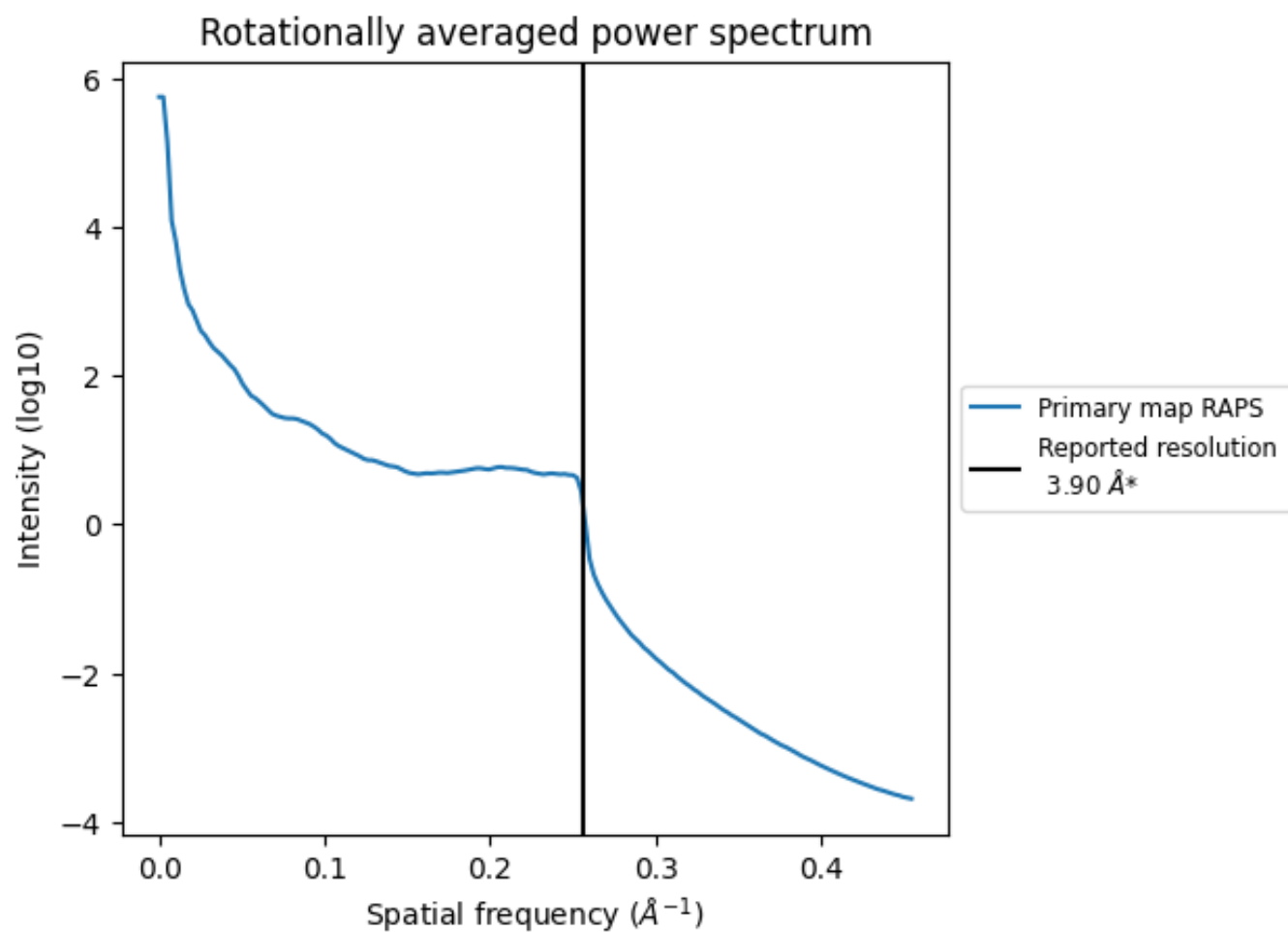
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 1789 nm³; this corresponds to an approximate mass of 1616 kDa.

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

6.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

7 Fourier-Shell correlation ⓘ

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

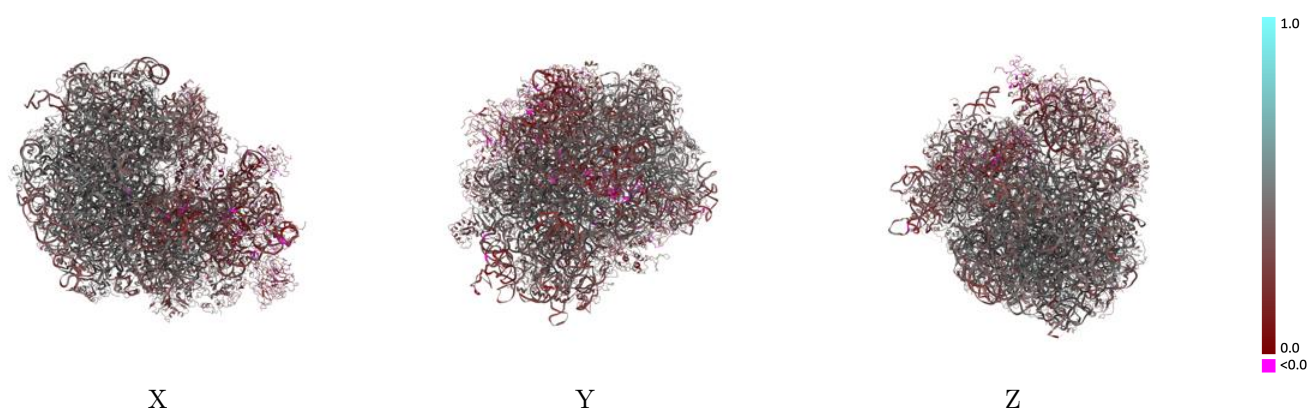
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0048 and PDB model 6GQB. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)

This section was not generated.

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

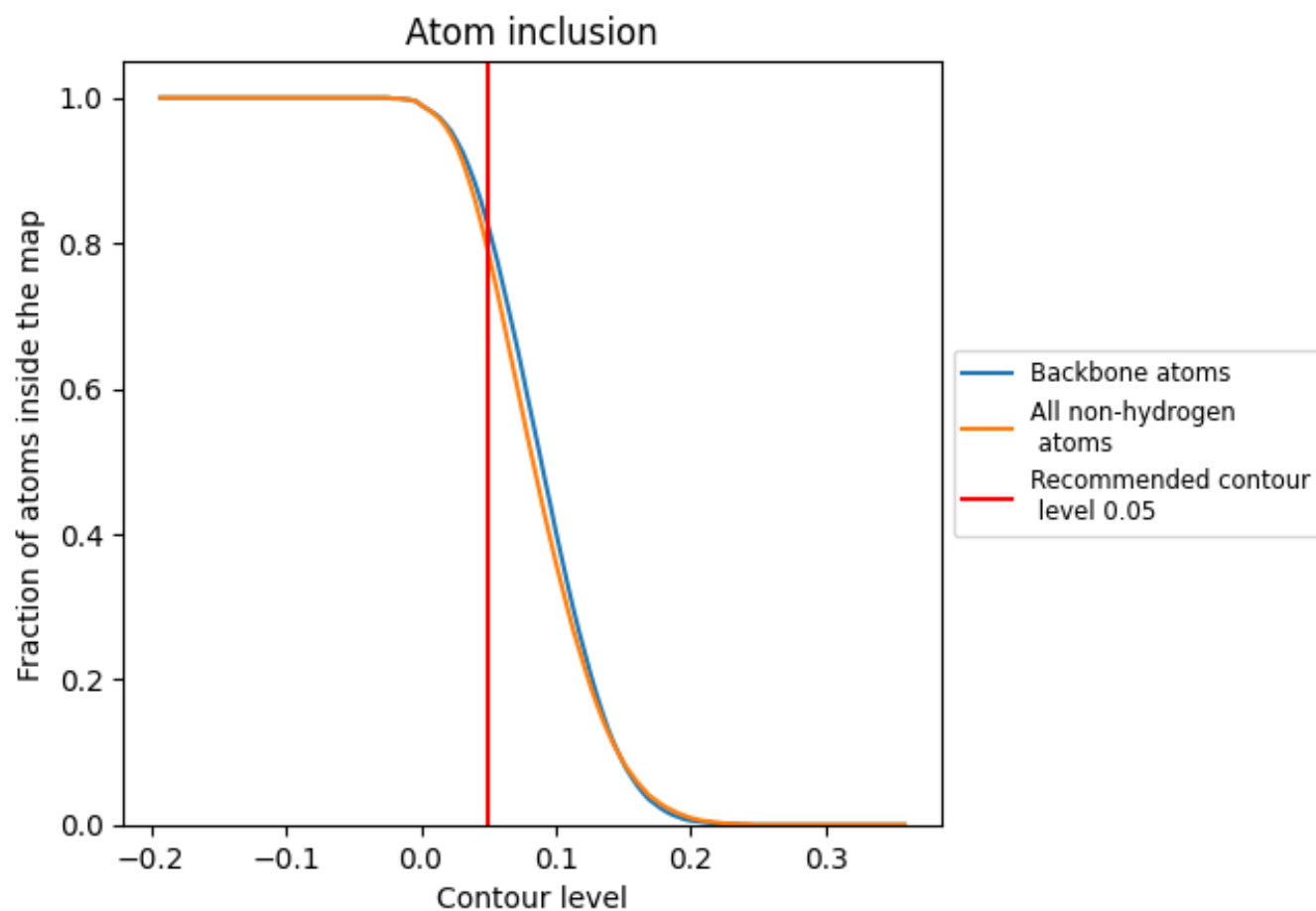


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7870	 0.3860
1	 0.9090	 0.4170
2	 0.8330	 0.3500
3	 0.9370	 0.4000
4	 0.9270	 0.4290
A	 0.7650	 0.4780
AA	 0.6330	 0.2540
AB	 0.6340	 0.4200
AC	 0.0930	 0.1310
AD	 0.7520	 0.4160
AE	 0.7800	 0.4120
AF	 0.6210	 0.2940
AG	 0.5360	 0.2490
AH	 0.5530	 0.2950
AI	 0.6010	 0.3030
AJ	 0.5830	 0.2620
AK	 0.4630	 0.2710
AL	 0.7270	 0.3860
AM	 0.7320	 0.4320
AN	 0.6860	 0.4300
AO	 0.7230	 0.3440
AP	 0.3310	 0.1820
AQ	 0.7100	 0.4060
AR	 0.7340	 0.3640
AS	 0.3730	 0.2350
AT	 0.6790	 0.3240
AU	 0.6190	 0.3780
AV	 0.4670	 0.2250
AW	 0.3610	 0.1930
AX	 0.7150	 0.2840
AY	 0.4170	 0.3360
AZ	 0.3200	 0.2650
B	 0.8010	 0.4530
BA	 0.4440	 0.2740
C	 0.8250	 0.4530



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
D	 0.7690	 0.3740
E	 0.8220	 0.4200
F	 0.8000	 0.4400
G	 0.8030	 0.4100
H	 0.7640	 0.4180
I	 0.7730	 0.4390
J	 0.7190	 0.3720
L	 0.8320	 0.4450
M	 0.8130	 0.4070
N	 0.8330	 0.4670
O	 0.7850	 0.4410
P	 0.8040	 0.4670
P0	 0.1990	 0.2200
P2	 0.2060	 0.2200
Q	 0.8260	 0.4670
R	 0.7700	 0.4340
S	 0.7790	 0.4420
T	 0.7960	 0.4520
U	 0.7850	 0.4150
V	 0.6930	 0.4590
W	 0.7340	 0.4460
X	 0.7830	 0.4410
Y	 0.8450	 0.4590
Z	 0.8180	 0.4320
a	 0.8330	 0.4580
b	 0.7590	 0.4310
c	 0.8030	 0.4260
d	 0.7640	 0.4500
e	 0.7920	 0.4720
f	 0.8210	 0.4850
g	 0.7810	 0.4600
h	 0.8200	 0.4320
i	 0.7870	 0.4100
j	 0.8760	 0.5050
k	 0.7150	 0.4020
l	 0.8100	 0.4560
m	 0.7700	 0.4340
n	 0.6600	 0.4620
o	 0.7560	 0.4480
p	 0.7630	 0.4760
q	 0.6970	 0.3590
r	 0.7240	 0.3790

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
s	 0.6940	 0.3960
t	 0.5010	 0.2560
u	 0.7080	 0.3760
v	 0.4450	 0.2560
w	 0.6620	 0.3180
x	 0.7220	 0.3530
y	 0.7210	 0.3890
z	 0.7410	 0.3760