



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:35 AM UTC

PDB ID : 8Y5K / pdb_00008y5k
EMDB ID : EMD-38940
Title : E.coli transcription translation coupling complex in TTC-A state 2 containing mRNA with 27-mer spacer, NusG, NusA, fMet-tRNA(iMet), Phe-tRNA(Phe), and viomycin
Authors : Zhang, J.; Lu, G.; Wang, C.; Lin, J.
Deposited on : 2024-01-31
Resolution : 6.90 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

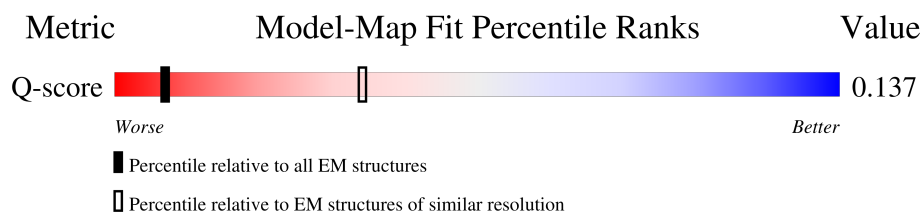
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.90 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	479 (6.40 - 7.40)

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

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 179757 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 L31.

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

- Molecule 2 is a protein called 50S ribosomal protein L32.

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

- Molecule 3 is a protein called 50S ribosomal protein L33.

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

- Molecule 4 is a protein called 50S ribosomal protein L34.

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

- Molecule 5 is a protein called 50S ribosomal protein L35.

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

- Molecule 6 is a protein called 50S ribosomal protein L36.

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

- Molecule 7 is a protein called 30S ribosomal protein S2.

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

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	206	Total	C	N	O	S	0	0
			1620	1025	304	288	3		

- Molecule 9 is a protein called 30S ribosomal protein S4.

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

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	157	Total	C	N	O	S	0	0
			1152	717	218	211	6		

- Molecule 11 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

- Molecule 12 is a protein called 30S ribosomal protein S7.

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

- Molecule 13 is a protein called 30S ribosomal protein S8.

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

- Molecule 14 is a protein called 30S ribosomal protein S9.

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

- Molecule 15 is a protein called 30S ribosomal protein S10.

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

- Molecule 16 is a protein called 30S ribosomal protein S11.

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

- Molecule 17 is a protein called 30S ribosomal protein S12.

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

- Molecule 18 is a protein called 30S ribosomal protein S13.

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

- Molecule 19 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 20 is a protein called 30S ribosomal protein S15.

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

- Molecule 21 is a protein called 30S ribosomal protein S16.

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

- Molecule 22 is a protein called 30S ribosomal protein S17.

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

- Molecule 23 is a protein called 30S ribosomal protein S18.

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

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

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

- Molecule 26 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	u	102	Total	C	N	O		0	0
			776	489	146	141			

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

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

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 1929590828

- Molecule 52 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	U	conflict	GB NR_103249

- Molecule 53 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	18	Total	C	N	O	P	0	0
			387	172	67	130	18		

- Molecule 55 is a DNA chain called templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	27	Total	C	N	O	P	0	0
			539	257	88	167	27		

- Molecule 56 is a DNA chain called non-templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	9	20	Total	C	N	O	P	0	0
			417	195	84	118	20		

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	A1	218	Total	C	N	O	S	0	0
			1677	1048	297	326	6		
57	A2	221	Total	C	N	O	S	0	0
			1698	1060	299	333	6		

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B1	1335	Total	C	N	O	S	0	0
			10353	6509	1842	1955	47		

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B2	1340	Total	C	N	O	S	0	0
			10496	6580	1833	2040	43		

- Molecule 60 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	W0	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 61 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	NG	88	Total	C	N	O	0	0
			433	257	88	88		

- Molecule 62 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
62	5	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 63 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
63	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 64 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	a	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 65 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	0	697	Total	C	N	O	S	0	0
			5399	3403	929	1042	25		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	705	GLY	-	expression tag	UNP P0A6M8
0	706	SER	-	expression tag	UNP P0A6M8
0	707	SER	-	expression tag	UNP P0A6M8
0	708	GLY	-	expression tag	UNP P0A6M8
0	709	HIS	-	expression tag	UNP P0A6M8
0	710	HIS	-	expression tag	UNP P0A6M8
0	711	HIS	-	expression tag	UNP P0A6M8
0	712	HIS	-	expression tag	UNP P0A6M8
0	713	HIS	-	expression tag	UNP P0A6M8
0	714	HIS	-	expression tag	UNP P0A6M8
0	715	HIS	-	expression tag	UNP P0A6M8
0	716	HIS	-	expression tag	UNP P0A6M8

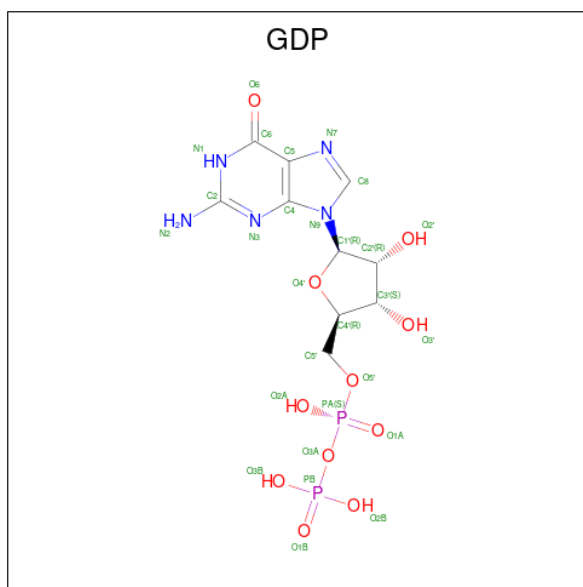
- Molecule 66 is a protein (with D amino acids) called Viomycin.

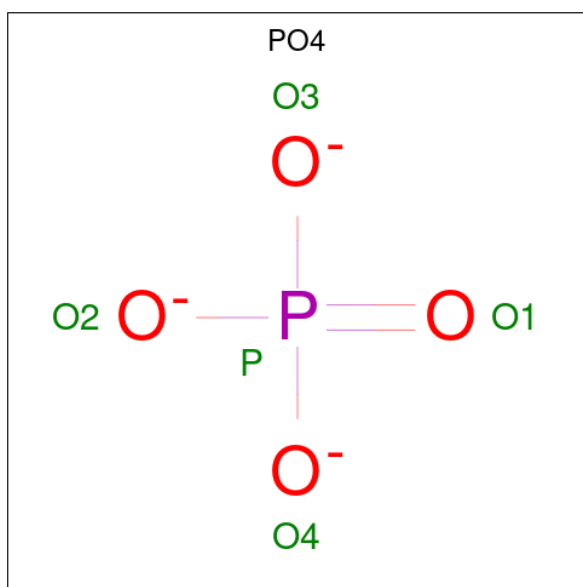
Mol	Chain	Residues	Atoms				AltConf	Trace
66	h	6	Total	C	N	O	0	0
			48	25	13	10		

- Molecule 67 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
67	B1	1	Total	Mg	0
			1	1	

- Molecule 68 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
69	0	1	5	4	1	0

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

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	626298	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	753.60004, 753.60004, 753.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.57, 1.57, 1.57	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](#)

4 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	$\# Z > 2$
66	UAL	h	5	66	6,8,9	2.36	2 (33%)	4,9,11	1.87	1 (25%)
66	5OH	h	6	66	7,12,13	0.73	0	4,16,18	1.32	1 (25%)
66	DPP	h	2	66	4,5,6	0.50	0	1,5,7	0.07	0
66	KBE	h	1	66	8,8,9	0.58	0	6,8,10	1.18	0

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
66	UAL	h	5	66	-	0/3/7/9	-
66	5OH	h	6	66	-	0/2/18/20	0/1/1/1
66	DPP	h	2	66	-	0/2/4/6	-
66	KBE	h	1	66	-	0/7/7/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	h	5	UAL	C1-N1	-4.94	1.32	1.40
66	h	5	UAL	C-CA	-2.84	1.40	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	h	5	UAL	O-C-CA	-3.29	121.27	125.39
66	h	6	5OH	CR-CB-CA	-2.37	110.09	112.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
69	PO4	0	802	-	4,4,4	1.15	0	6,6,6	0.73	0
68	GDP	0	801	-	29,30,30	1.13	4 (13%)	45,47,47	1.76	6 (13%)

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
68	GDP	0	801	-	-	0/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	0	801	GDP	C5-C4	2.86	1.46	1.38
68	0	801	GDP	C6-N1	-2.52	1.34	1.38
68	0	801	GDP	C5-N7	-2.28	1.34	1.39
68	0	801	GDP	C4-N9	-2.17	1.32	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	0	801	GDP	C5-C4-N3	-5.59	119.50	128.39
68	0	801	GDP	C2-N3-C4	4.92	120.77	112.30
68	0	801	GDP	N9-C4-N3	3.96	133.87	125.95
68	0	801	GDP	C6-C5-N7	3.54	136.74	130.29
68	0	801	GDP	C4-C5-N7	-2.54	106.64	110.67
68	0	801	GDP	O6-C6-C5	-2.36	120.29	126.53

There are no chirality outliers.

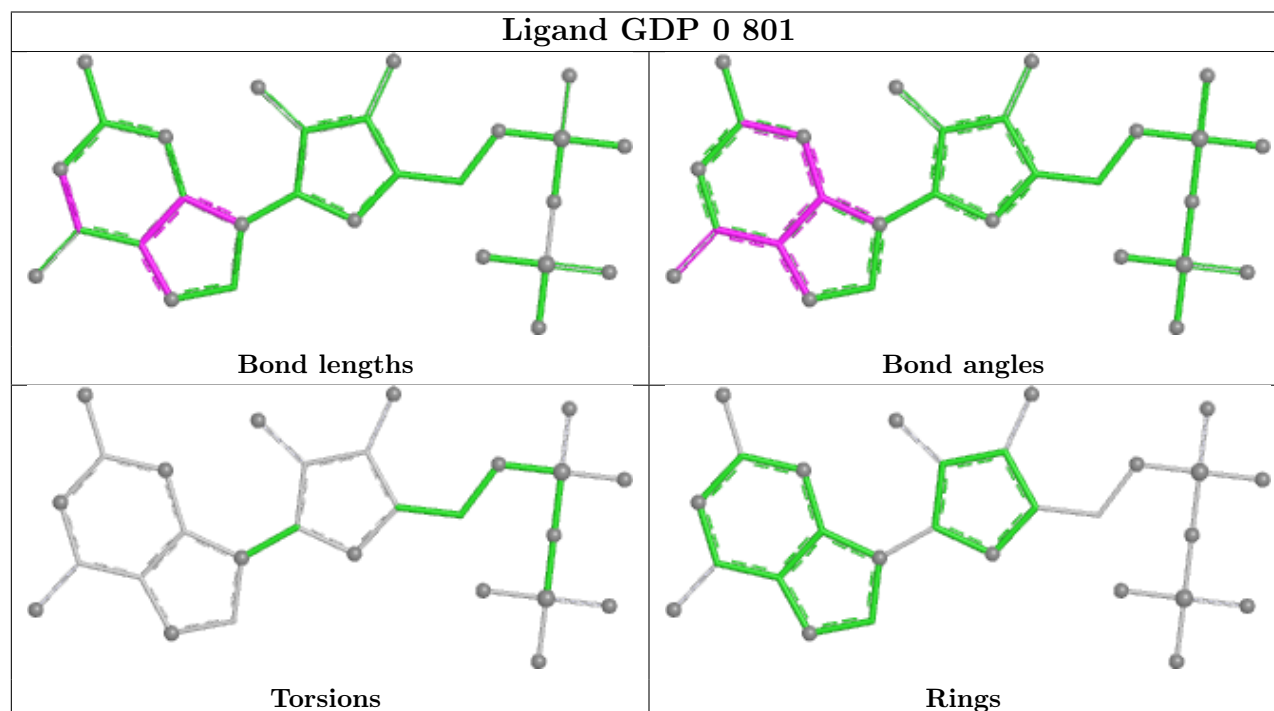
There are no torsion outliers.

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 [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

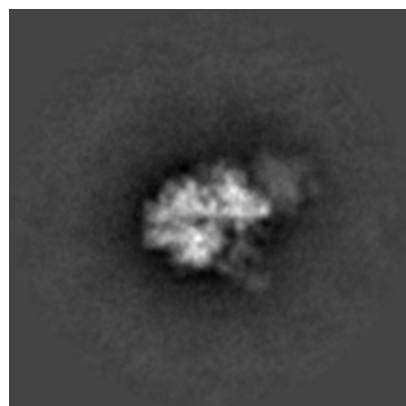
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38940. These allow visual inspection of the internal detail of the map and identification of artifacts.

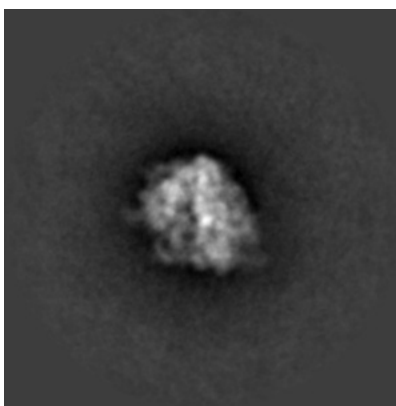
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

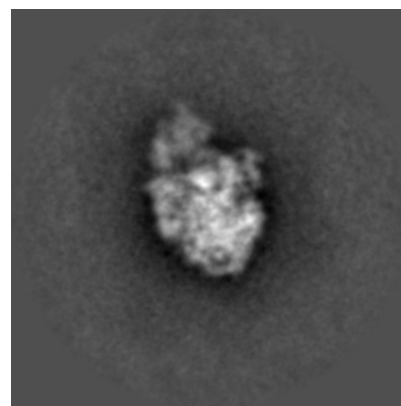
5.1.1 Primary map



X

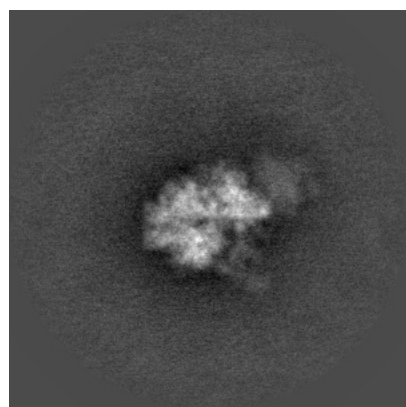


Y

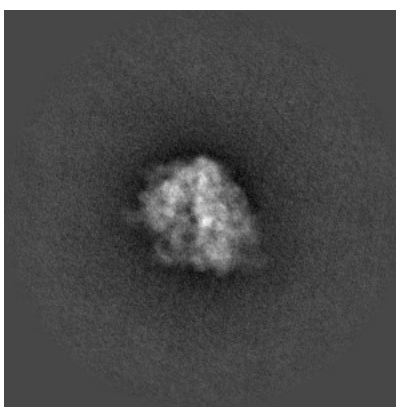


Z

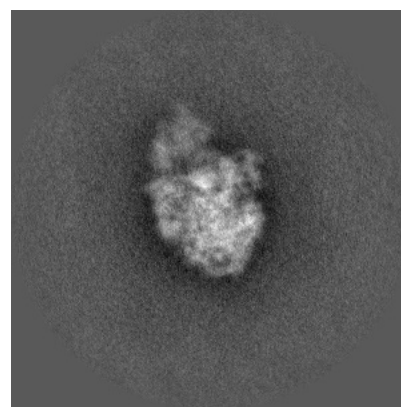
5.1.2 Raw map



X



Y

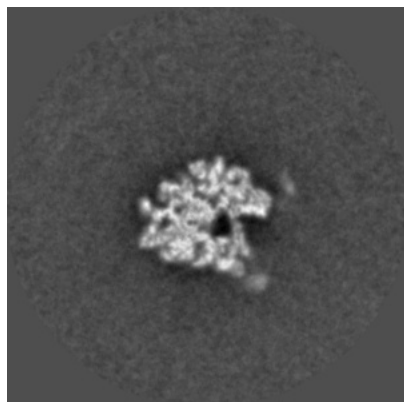


Z

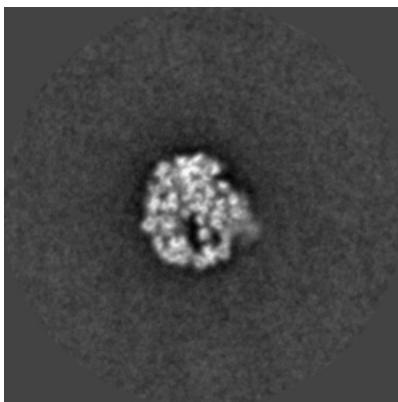
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

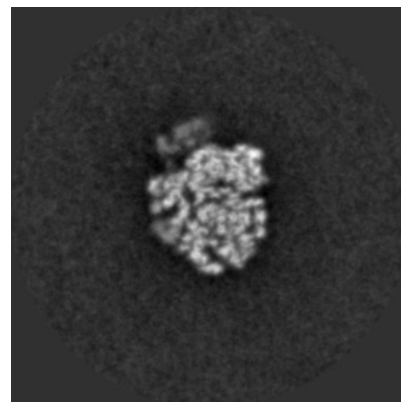
5.2.1 Primary map



X Index: 240

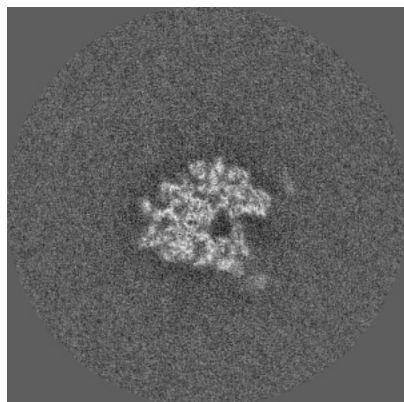


Y Index: 240

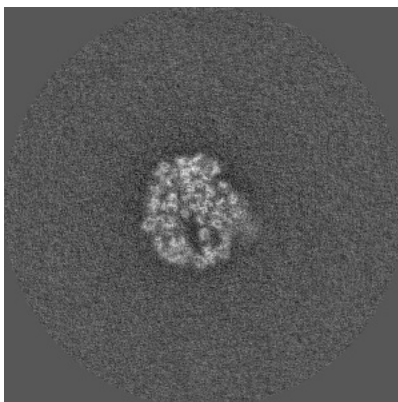


Z Index: 240

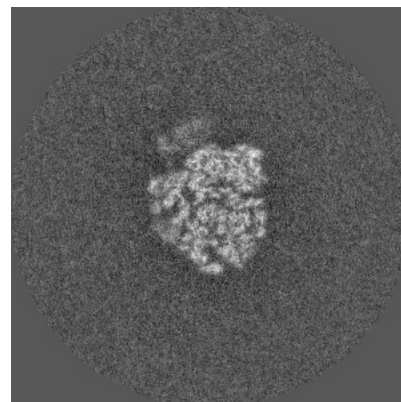
5.2.2 Raw map



X Index: 240



Y Index: 240

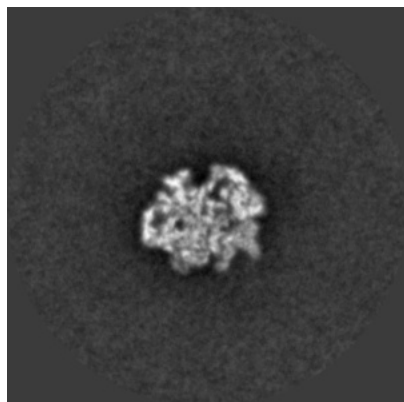


Z Index: 240

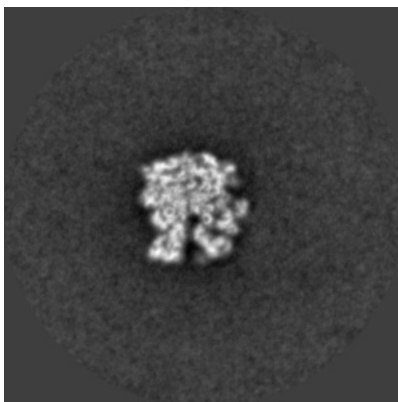
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

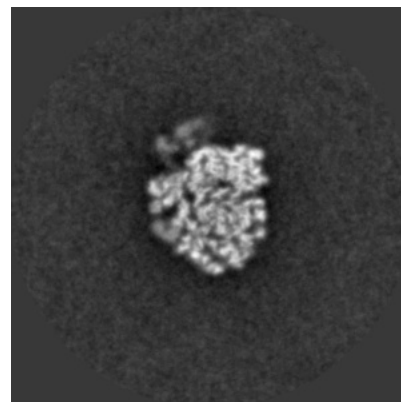
5.3.1 Primary map



X Index: 262

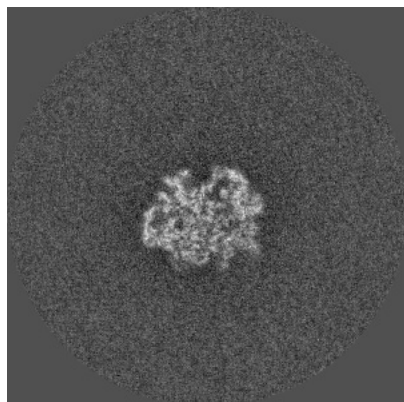


Y Index: 223

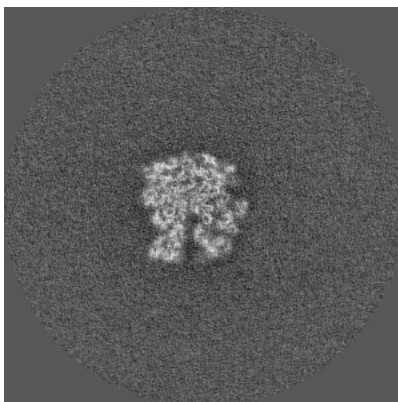


Z Index: 238

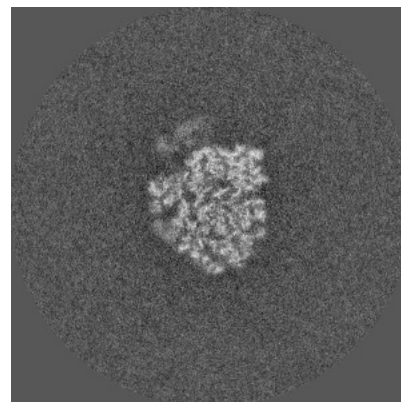
5.3.2 Raw map



X Index: 263



Y Index: 223

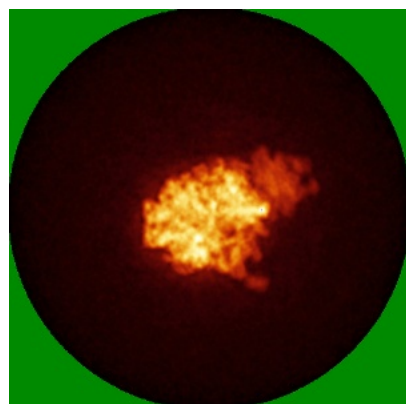


Z Index: 238

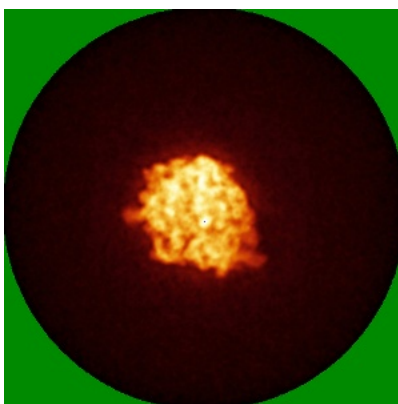
The images above show the largest variance slices of the map in three orthogonal directions.

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

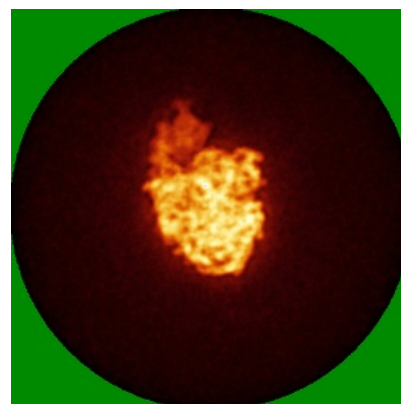
5.4.1 Primary map



X

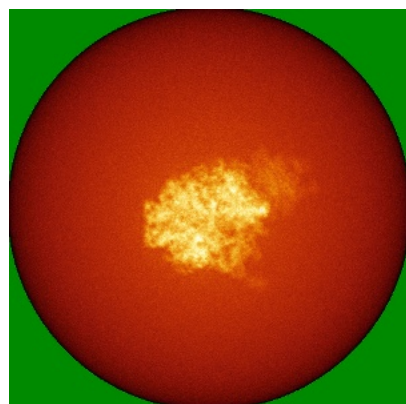


Y

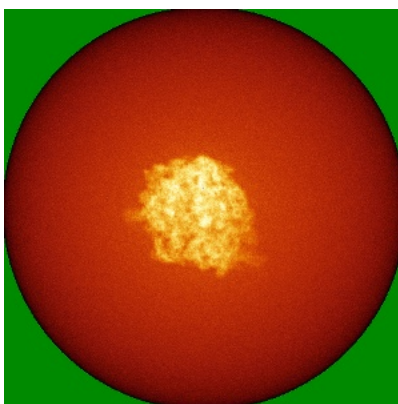


Z

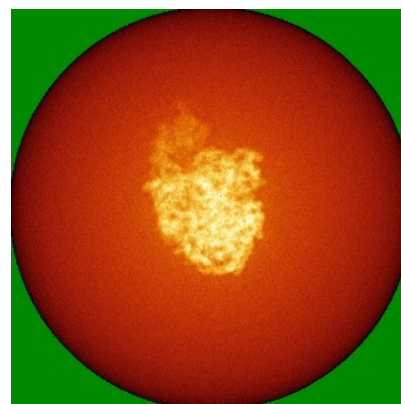
5.4.2 Raw map



X



Y

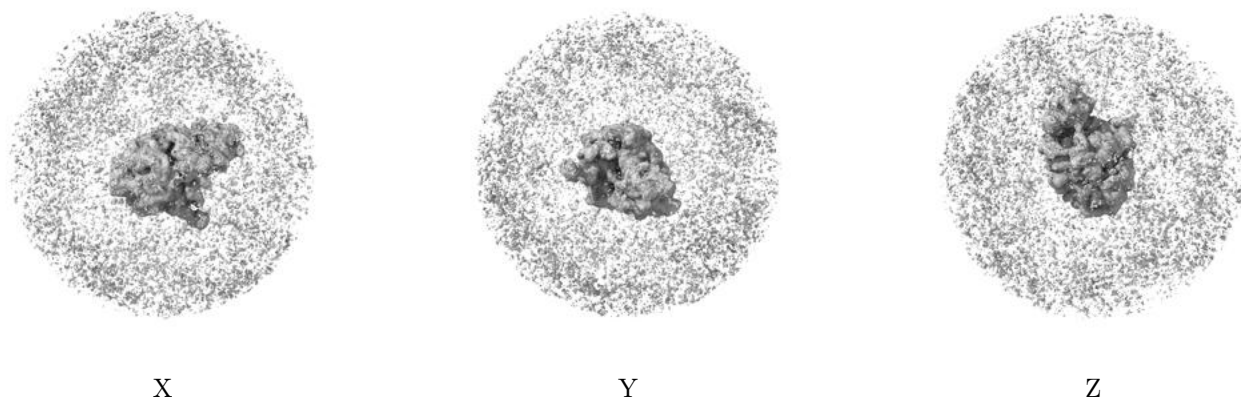


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

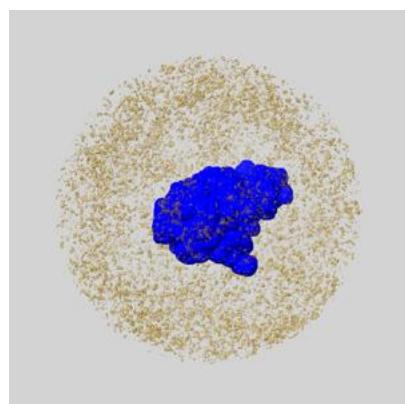
5.6 Mask visualisation [i](#)

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

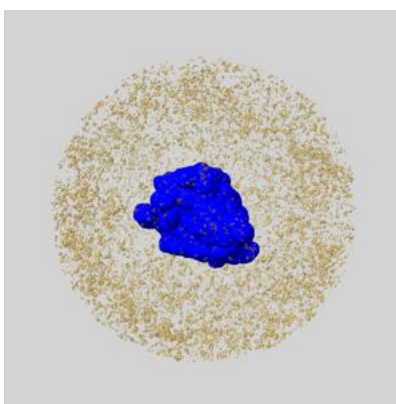
A mask typically either:

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

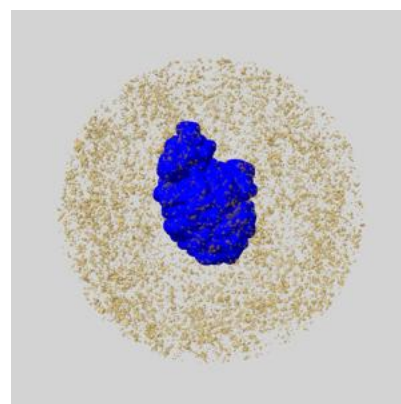
5.6.1 emd_38940_msk_1.map [i](#)



X



Y

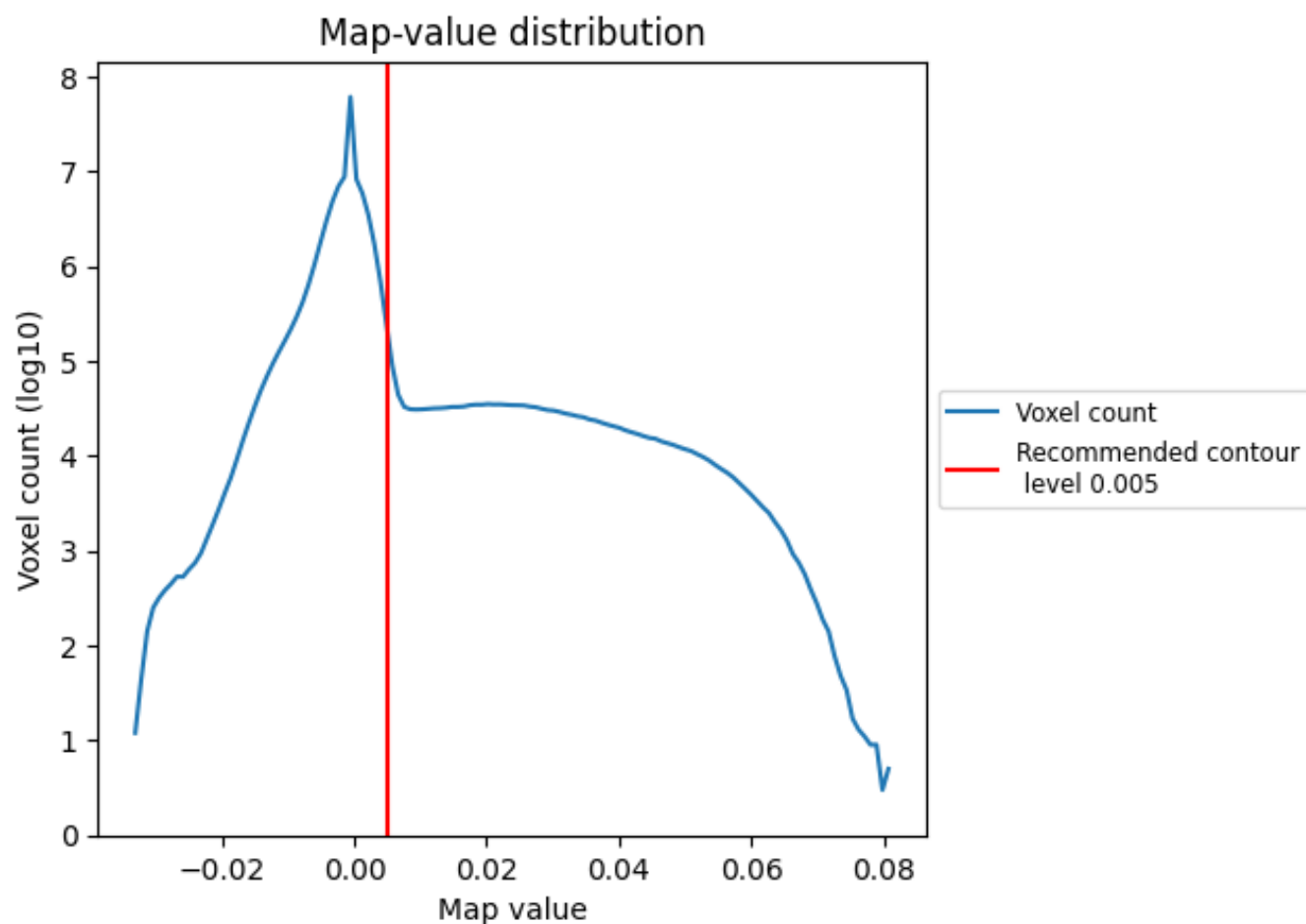


Z

6 Map analysis [i](#)

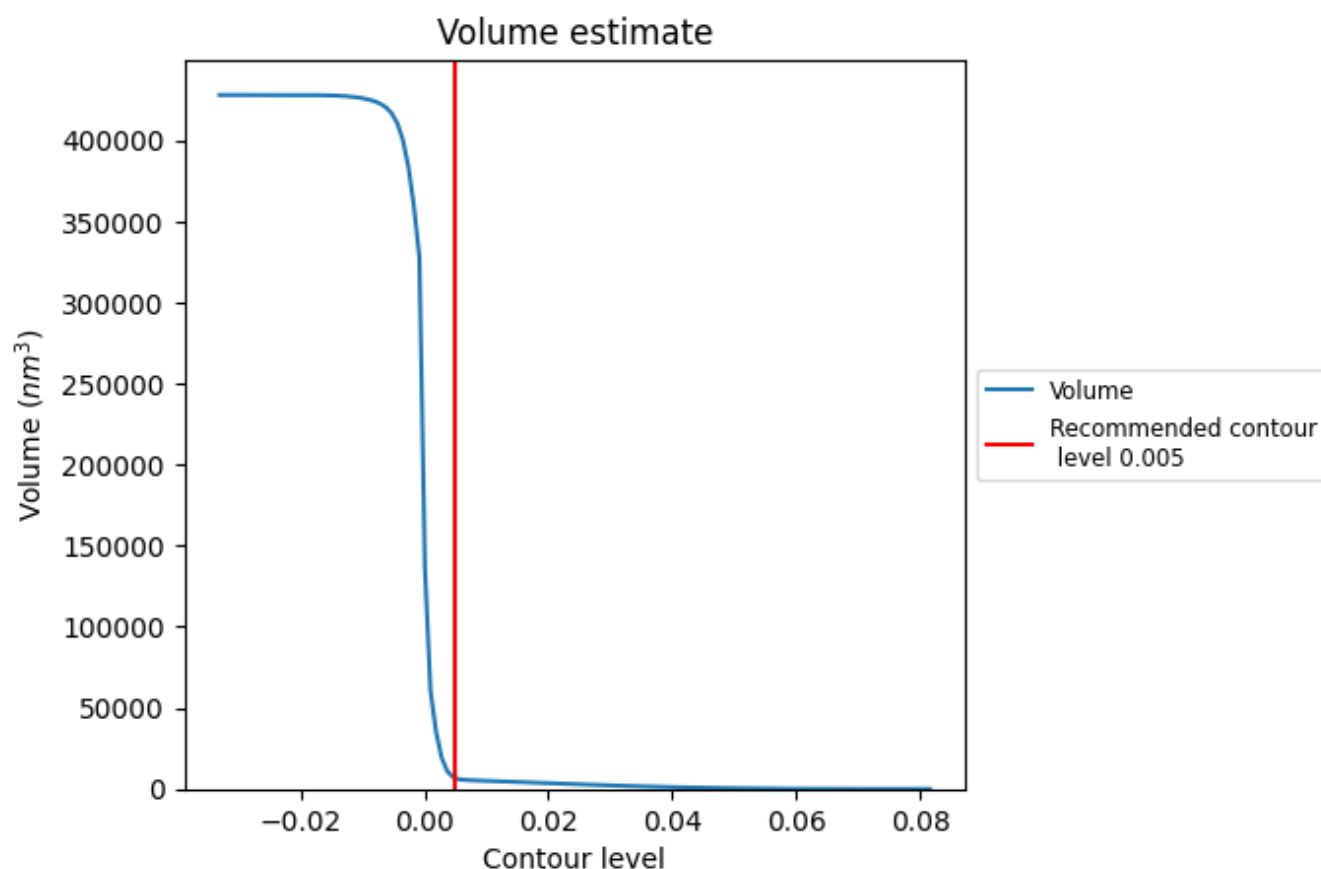
This section contains the results of statistical analysis of the map.

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.

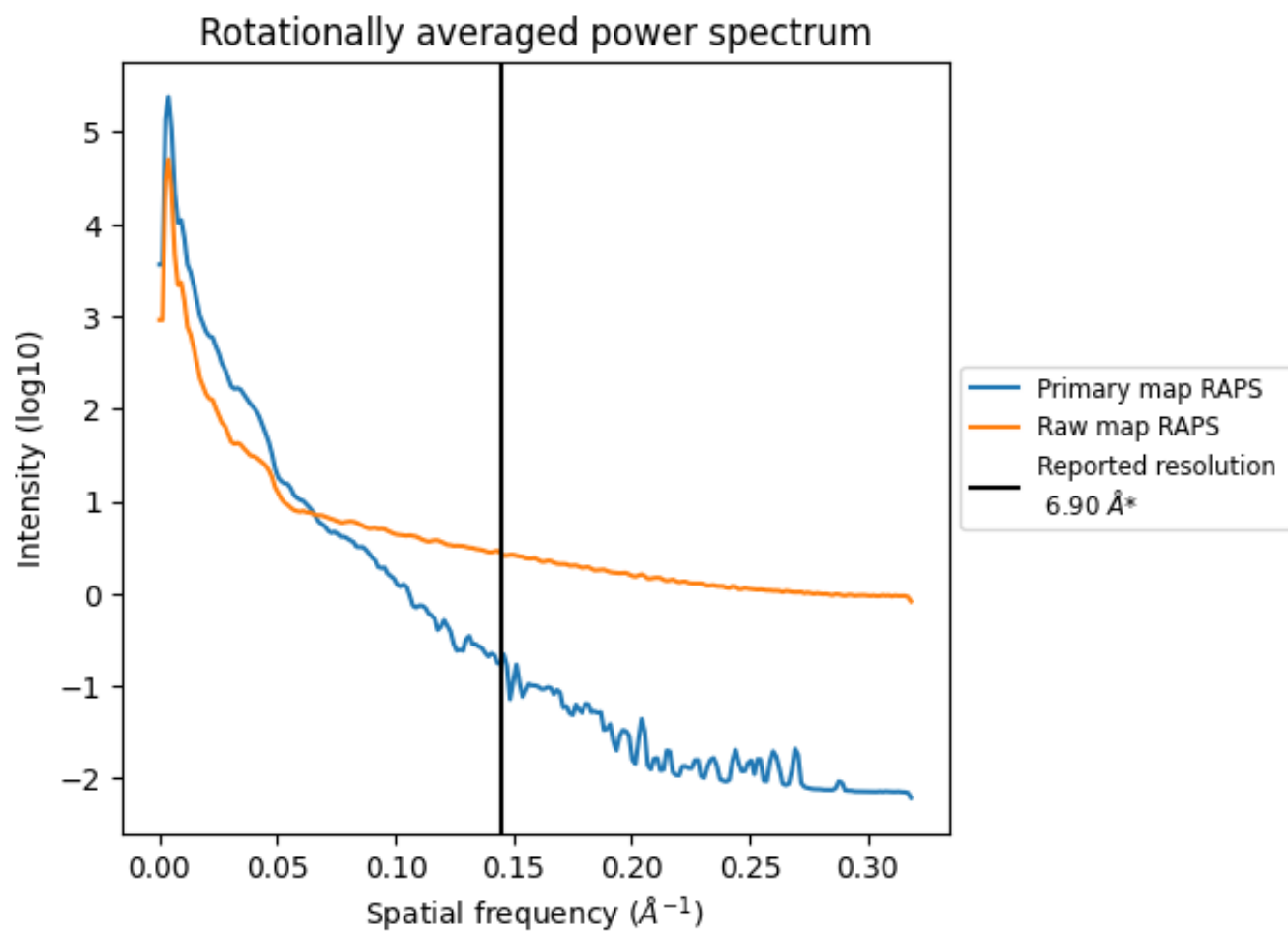
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 6757 nm^3 ; this corresponds to an approximate mass of 6104 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](#)

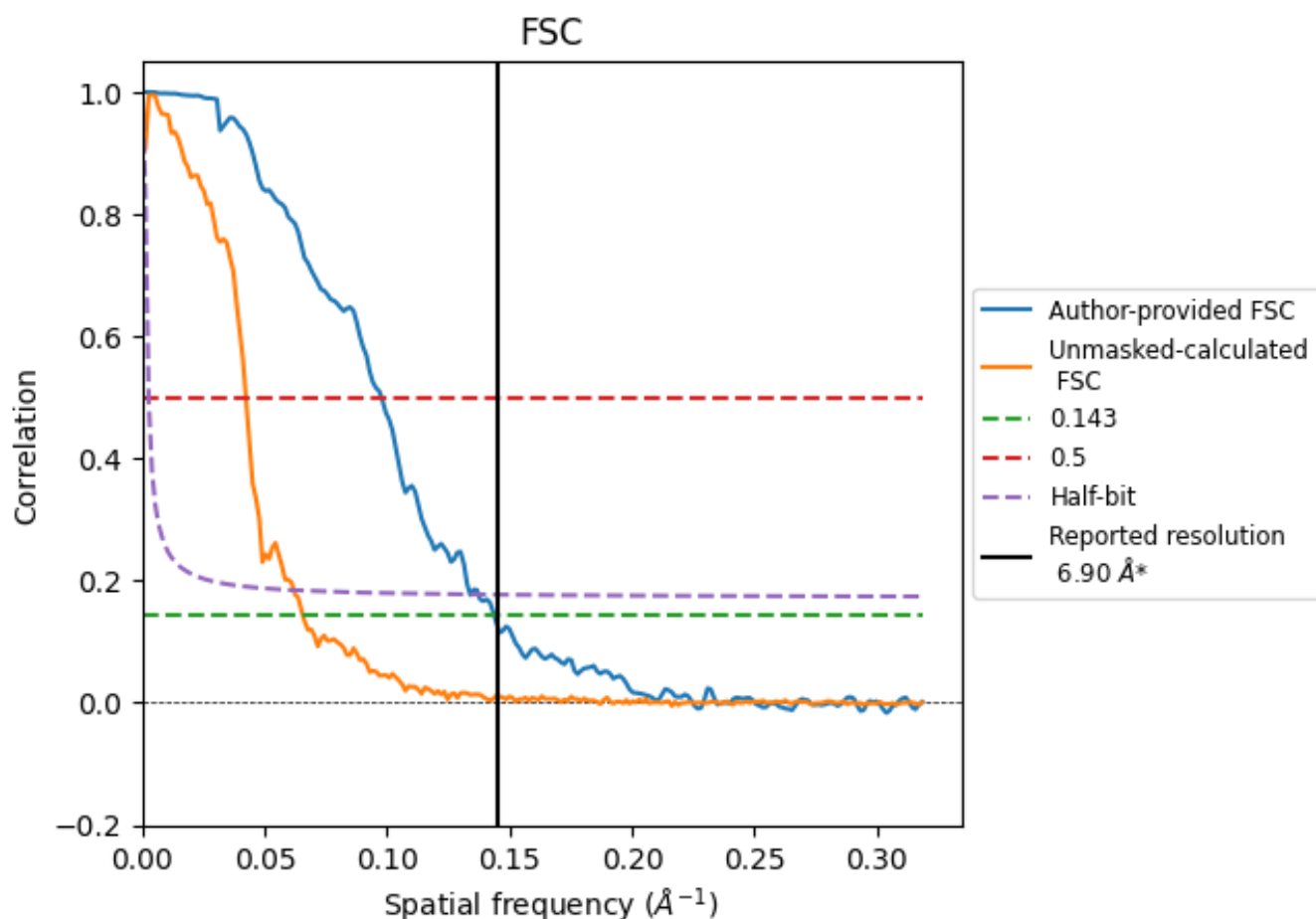


*Reported resolution corresponds to spatial frequency of 0.145 Å⁻¹

7 Fourier-Shell correlation [i](#)

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

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.145 Å⁻¹

7.2 Resolution estimates [i](#)

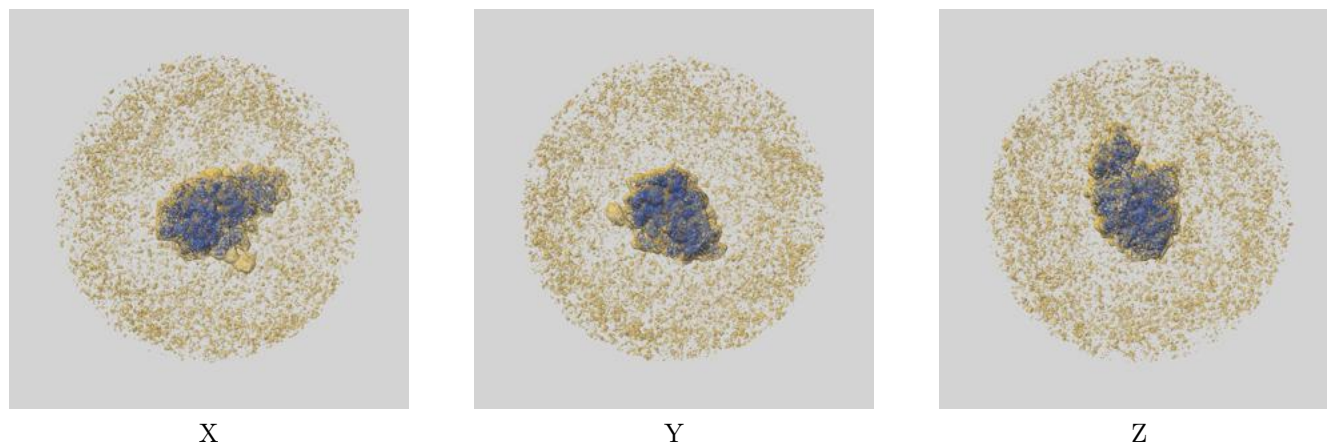
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.90	-	-
Author-provided FSC curve	6.95	10.24	7.46
Unmasked-calculated*	15.22	23.64	16.16

*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 15.22 differs from the reported value 6.9 by more than 10 %

8 Map-model fit [i](#)

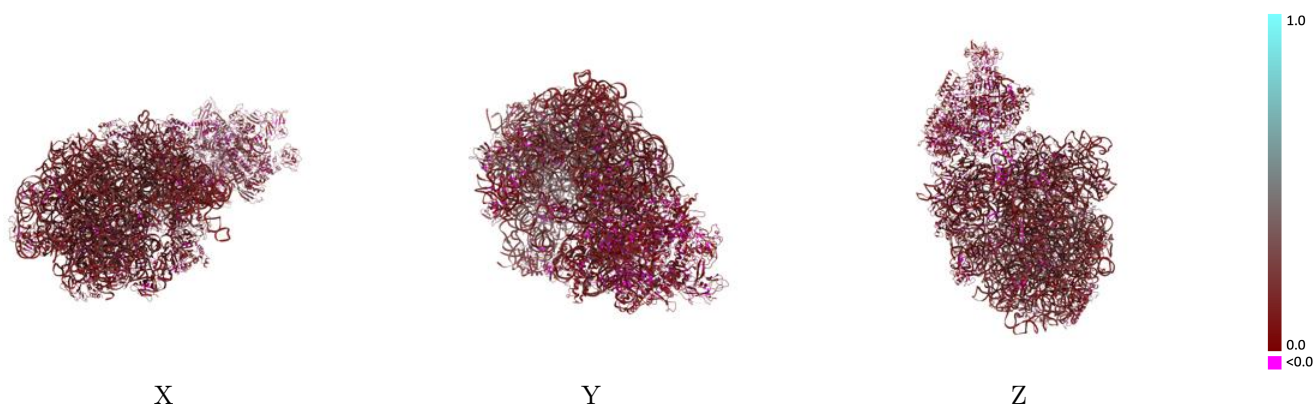
This section contains information regarding the fit between EMDB map EMD-38940 and PDB model 8Y5K. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



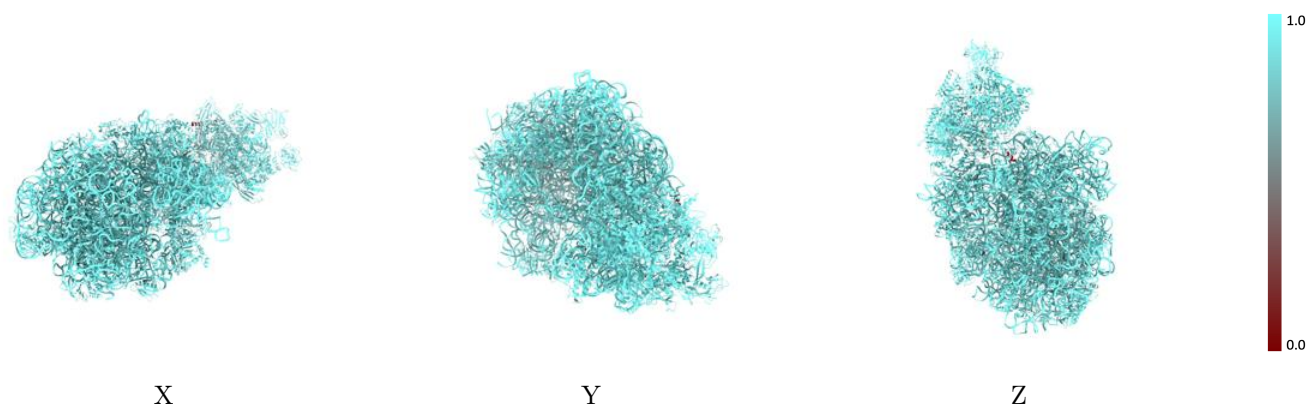
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



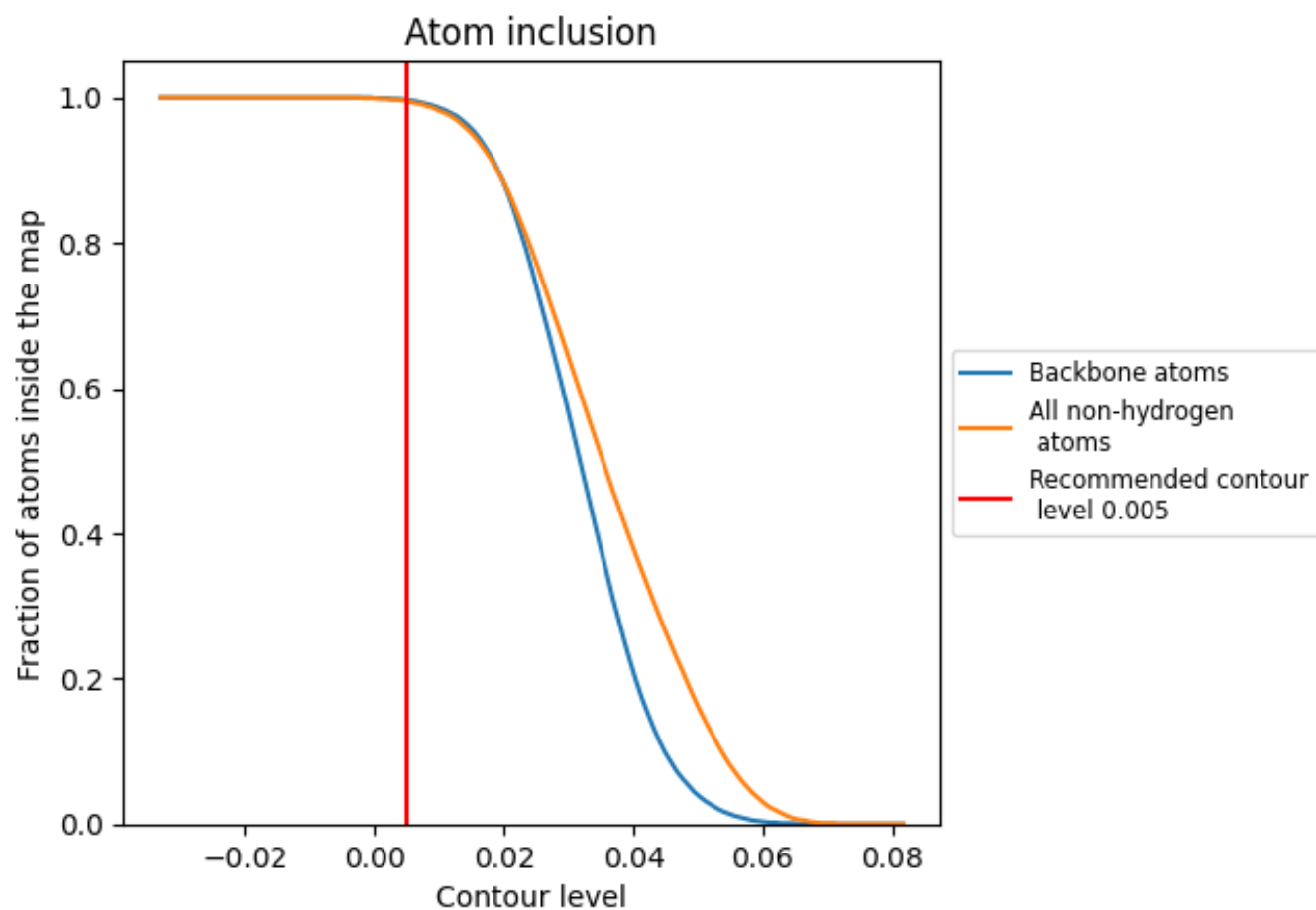
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.005).

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

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9950	 0.1370
0	 0.9740	 0.1210
1	 1.0000	 0.1650
2	 1.0000	 0.1430
3	 1.0000	 0.1560
4	 1.0000	 0.1610
5	 0.9990	 0.1110
6	 0.9970	 0.1430
8	 1.0000	 0.1480
9	 1.0000	 0.1360
A	 0.9710	 0.0770
A1	 0.9900	 0.1070
A2	 0.9970	 0.1060
B	 1.0000	 0.0900
B1	 0.9880	 0.1060
B2	 0.9870	 0.0970
C	 0.9830	 0.0980
D	 0.9920	 0.0780
E	 1.0000	 0.0690
F	 1.0000	 0.0830
G	 0.9990	 0.1160
H	 0.9930	 0.1260
I	 0.9990	 0.1050
J	 0.9980	 0.1210
K	 0.9890	 0.1230
L	 0.9850	 0.1180
M	 0.9950	 0.1150
N	 0.9980	 0.0880
NG	 1.0000	 0.1490
O	 0.9990	 0.1010
P	 0.9990	 0.1250
Q	 0.9630	 0.1070
R	 0.9990	 0.1290
S	 1.0000	 0.0990
T	 0.9990	 0.1140



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Chain	Atom inclusion	Q-score
U	 1.0000	 0.1040
V	 0.9970	 0.1090
W	 1.0000	 0.1070
W0	 0.6910	 0.0270
X	 1.0000	 0.1030
Y	 0.9970	 0.1150
Z	 0.9850	 0.1060
a	 0.9930	 0.0730
b	 0.9940	 0.1240
c	 0.9940	 0.1070
d	 0.9970	 0.1100
e	 0.9790	 0.1070
f	 0.9960	 0.1110
g	 0.9390	 0.1060
h	 1.0000	 0.1450
i	 0.9920	 0.0860
j	 0.9990	 0.1100
k	 0.9890	 0.1430
l	 0.9980	 0.0860
m	 0.9960	 0.1220
n	 0.9990	 0.0980
o	 1.0000	 0.1050
p	 0.9890	 0.1370
q	 1.0000	 0.1070
r	 1.0000	 0.0990
s	 0.9990	 0.1160
t	 0.9960	 0.0920
u	 0.9990	 0.0980
v	 0.9990	 0.1030
w	 1.0000	 0.0880
x	 1.0000	 0.1150
y	 0.9980	 0.1170
z	 1.0000	 0.1140