



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 07:22 PM UTC

PDB ID : 9IT2 / pdb_00009it2
EMDB ID : EMD-60854
Title : Cryo-EM structure of urease from *Ureaplasma parvum*
Authors : Fujita, J.; Namba, K.; Wu, H.N.; Yanagihara, I.
Deposited on : 2024-07-19
Resolution : 2.03 Å (reported)
Based on initial model : .

This is a wwPDB EM Validation Summary 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:

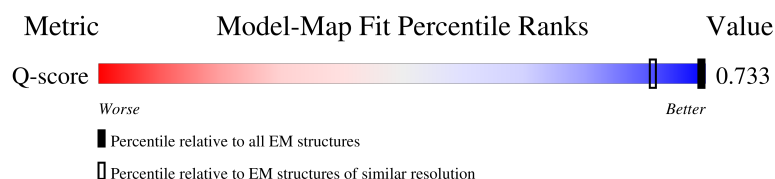
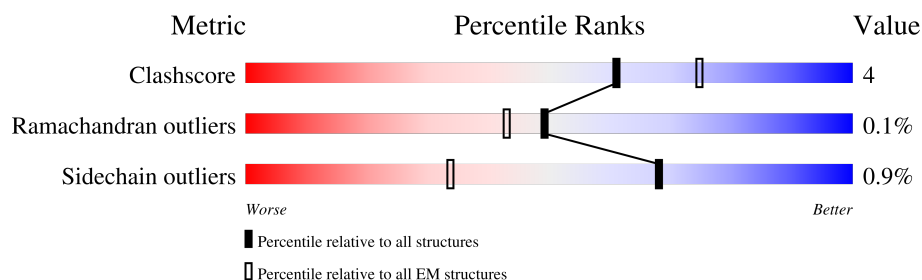
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1771 (1.55 - 2.53)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	101	 92% 8%
1	D	101	 89% 11%
1	G	101	 92% 8%
2	B	124	 81% 11% 8%

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Mol	Chain	Length	Quality of chain
2	E	124	 83%9%8%
2	H	124	 81%11%8%
3	C	598	 87%13%
3	F	598	 89%11%
3	I	598	 89%11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19091 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 Urease subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	101	Total	C	N	O	S	1	0
			792	496	141	149	6		
1	D	101	Total	C	N	O	S	1	0
			792	496	141	149	6		
1	G	101	Total	C	N	O	S	1	0
			792	496	141	149	6		

- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	114	Total	C	N	O	S	0	0
			884	559	159	165	1		
2	E	114	Total	C	N	O	S	0	0
			884	559	159	165	1		
2	H	114	Total	C	N	O	S	0	0
			884	559	159	165	1		

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	598	Total	C	N	O	S	0	0
			4537	2867	763	883	24		
3	F	598	Total	C	N	O	S	0	0
			4537	2867	763	883	24		
3	I	598	Total	C	N	O	S	0	0
			4537	2867	763	883	24		

- Molecule 4 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	O	S	0
			4	2	1	1	
4	F	1	Total	C	O	S	0
			4	2	1	1	
4	I	1	Total	C	O	S	0
			4	2	1	1	

- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	2	Total	Ni	0
			2	2	
5	F	2	Total	Ni	0
			2	2	
5	I	2	Total	Ni	0
			2	2	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	25	Total	O	0
			25	25	
6	B	5	Total	O	0
			5	5	
6	C	118	Total	O	0
			118	118	

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Mol	Chain	Residues	Atoms		AltConf
6	D	27	Total 27	O 27	0
6	E	8	Total 8	O 8	0
6	F	109	Total 109	O 109	0
6	G	22	Total 22	O 22	0
6	H	5	Total 5	O 5	0
6	I	115	Total 115	O 115	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Urease subunit gamma

Chain A:  92% 8%



- Molecule 1: Urease subunit gamma

Chain D:  89% 11%




- Molecule 1: Urease subunit gamma

Chain G:  92% 8%




- Molecule 2: Urease subunit beta

Chain B:  81% 11% 8%

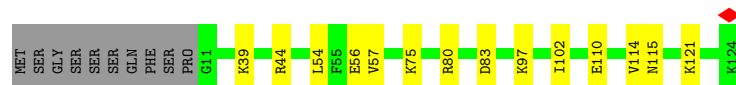


- Molecule 2: Urease subunit beta

Chain E:  83% 9% 8%



- Molecule 2: Urease subunit beta



Category	Item	Value
A	A287	100
	A288	100
	A289	100
	A290	100
	A291	100
	A292	100
	A293	100
	A294	100
	A295	100
	A296	100
B	B307	100
	B308	100
	B309	100
	B310	100
	B311	100
	B312	100
	B313	100
	B314	100
	B315	100
	B316	100
C	C323	100
	C324	100
	C325	100
	C326	100
	C327	100
	C328	100
	C329	100
	C330	100
	C331	100
	C332	100
D	D332	100
	D333	100
	D334	100
	D335	100
	D336	100
	D337	100
	D338	100
	D339	100
	D340	100
	D341	100
E	E356	100
	E357	100
	E358	100
	E359	100
	E360	100
	E361	100
	E362	100
	E363	100
	E364	100
	E365	100
F	F371	100
	F372	100
	F373	100
	F374	100
	F375	100
	F376	100
	F377	100
	F378	100
	F379	100
	F380	100
G	G386	100
	G387	100
	G388	100
	G389	100
	G390	100
	G391	100
	G392	100
	G393	100
	G394	100
	G395	100
H	H421	100
	H422	100
	H423	100
	H424	100
	H425	100
	H426	100
	H427	100
	H428	100
	H429	100
	H430	100
I	I437	100
	I438	100
	I439	100
	I440	100
	I441	100
	I442	100
	I443	100
	I444	100
	I445	100
	I446	100
J	J454	100
	J455	100
	J456	100
	J457	100
	J458	100
	J459	100
	J460	100
	J461	100
	J462	100
	J463	100
K	K462	100
	K463	100
	K464	100
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L	L478	100
	L479	100
	L480	100
	L481	100
	L482	100
	L483	100
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M	M496	100
	M497	100
	M498	100
	M499	100
	M500	100
	M501	100
	M502	100
	M503	100
	M504	100
	M505	100
N	N511	100
	N512	100
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	N514	100
	N515	100
	N516	100
	N517	100
	N518	100
	N519	100
	N520	100
O	O524	100
	O525	100
	O526	100
	O527	100
	O528	100
	O529	100
	O530	100
	O531	100
	O532	100
	O533	100
P	P539	100
	P540	100
	P541	100
	P542	100
	P543	100

L540	L549	L560	L567	F598	Y310	D320	K323	V324	C325	H326	H327	L328	N329	P330	K331	V332	P333	E334	D336	V336	A337	F338	A339	D340	S341	S361	I362	K363	S364	S365	D366	G371	R372	R379	M383	K386	L394	Y409	D437	V454	K455	C462	P467	R488	Y511	K512	L513	M1	F45	S69	K66	E71	L138	L145	T160	G167	M168	K185	K203	G206	K223	L224	H225	E226	D227	W228	L251	H252	T253	F261	T265	W269	Y277	H278	T279	G284	A287	P288	D289	T293	T304	N305	P306	T307	I308	P309
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Category	Item	Value
L	L560	10
	L567	10
	L586	10
	F598	10
	T307	10
	T308	10
	P309	10
	Y310	10
	T311	10
	L322	10
M	M1	10
	F45	10
	S59	10
	L138	10
	V152	10
	T160	10
	M168	10
	G171	10
	P179	10
	K185	10
D	D192	10
	K203	10
	G206	10
	K223	10
	L224	10
	H225	10
	E226	10
	D227	10
	M228	10
	T251	10
T	T252	10
	T253	10
	D254	10
	E258	10
	F261	10
	T274	10
	Y277	10
	H278	10
	T279	10
	A287	10
P	P288	10
	T293	10
	T299	10
	L300	10
	P301	10
	T304	10
	N305	10
	P306	10
	A339	10
	D	D340
S341		10
R342		10
L343		10
T360		10
M363		10
S364		10
S365		10
D366		10
M370		10
G	G371	10
	R372	10
	R379	10
	K386	10
	M387	10
	K455	10
	L478	10
	V498	10
	P519	10
	K529	10
S	S530	10
	M531	10
	S535	10
	L540	10
	A549	10

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	207602	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.929	Depositor
Minimum map value	-1.557	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	314.28, 314.28, 314.28	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.873, 0.873, 0.873	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, NI, BME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/798	0.28	0/1075
1	D	0.12	0/798	0.27	0/1075
1	G	0.10	0/798	0.23	0/1075
2	B	0.08	0/899	0.25	0/1204
2	E	0.08	0/899	0.24	0/1204
2	H	0.10	0/899	0.27	0/1204
3	C	0.11	0/4612	0.32	0/6249
3	F	0.11	0/4612	0.31	0/6249
3	I	0.10	0/4612	0.30	0/6249
All	All	0.10	0/18927	0.30	0/25584

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	792	0	833	6	0
1	D	792	0	833	8	0
1	G	792	0	833	6	0
2	B	884	0	892	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	884	0	892	8	0
2	H	884	0	892	9	0
3	C	4537	0	4514	53	0
3	F	4537	0	4514	45	0
3	I	4537	0	4514	43	0
4	C	4	0	5	0	0
4	F	4	0	5	0	0
4	I	4	0	5	1	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
5	I	2	0	0	0	0
6	A	25	0	0	0	0
6	B	5	0	0	0	0
6	C	118	0	0	1	0
6	D	27	0	0	0	0
6	E	8	0	0	0	0
6	F	109	0	0	0	0
6	G	22	0	0	0	0
6	H	5	0	0	0	0
6	I	115	0	0	0	0
All	All	19091	0	18732	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 164 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:323:MET:HA	3:I:328:LEU:HB2	1.74	0.70
3:C:59:SER:HB2	3:F:206:GLY:HA2	1.74	0.69
3:C:206:GLY:HA2	3:I:59:SER:HB2	1.75	0.69
2:B:83:ASP:OD2	3:I:1:MET:N	2.29	0.66
3:F:59:SER:HB2	3:I:206:GLY:HA2	1.77	0.65

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	100/101 (99%)	100 (100%)	0	0	100	100
1	D	100/101 (99%)	100 (100%)	0	0	100	100
1	G	100/101 (99%)	100 (100%)	0	0	100	100
2	B	112/124 (90%)	107 (96%)	4 (4%)	1 (1%)	14	7
2	E	112/124 (90%)	106 (95%)	5 (4%)	1 (1%)	14	7
2	H	112/124 (90%)	108 (96%)	3 (3%)	1 (1%)	14	7
3	C	595/598 (100%)	576 (97%)	19 (3%)	0	100	100
3	F	595/598 (100%)	574 (96%)	21 (4%)	0	100	100
3	I	595/598 (100%)	576 (97%)	19 (3%)	0	100	100
All	All	2421/2469 (98%)	2347 (97%)	71 (3%)	3 (0%)	49	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	114	VAL
2	E	114	VAL
2	H	114	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/87 (101%)	87 (99%)	1 (1%)	65	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	88/87 (101%)	86 (98%)	2 (2%)	44	43
1	G	88/87 (101%)	87 (99%)	1 (1%)	65	68
2	B	93/102 (91%)	93 (100%)	0	100	100
2	E	93/102 (91%)	93 (100%)	0	100	100
2	H	93/102 (91%)	93 (100%)	0	100	100
3	C	482/482 (100%)	477 (99%)	5 (1%)	68	71
3	F	482/482 (100%)	479 (99%)	3 (1%)	78	79
3	I	482/482 (100%)	477 (99%)	5 (1%)	68	71
All	All	1989/2013 (99%)	1972 (99%)	17 (1%)	68	73

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	341	SER
3	I	531	MET
1	D	84	VAL
3	F	185	LYS
3	F	308	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	329	ASN
3	F	482	GLN
3	I	539	ASN
3	I	329	ASN
3	I	492	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 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
3	KCX	I	223	3,5	10,11,12	0.97	0	6,12,14	1.36	1 (16%)
3	KCX	F	223	3,5	10,11,12	0.97	0	6,12,14	1.31	1 (16%)
3	KCX	C	223	3,5	10,11,12	0.96	0	6,12,14	1.33	1 (16%)

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
3	KCX	I	223	3,5	-	1/9/10/12	-
3	KCX	F	223	3,5	-	1/9/10/12	-
3	KCX	C	223	3,5	-	1/9/10/12	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	223	KCX	OQ1-CX-NZ	-3.24	120.00	124.92
3	C	223	KCX	OQ1-CX-NZ	-3.17	120.10	124.92
3	F	223	KCX	OQ1-CX-NZ	-3.11	120.20	124.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	223	KCX	C-CA-CB-CG
3	F	223	KCX	C-CA-CB-CG
3	I	223	KCX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 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	$\# Z > 2$
4	BME	C	601	5	3,3,3	0.30	0	2,2,2	0.40	0
4	BME	F	601	5	3,3,3	0.31	0	2,2,2	0.37	0
4	BME	I	601	5	3,3,3	0.29	0	2,2,2	0.38	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
4	BME	C	601	5	-	0/1/1/1	-
4	BME	F	601	5	-	1/1/1/1	-
4	BME	I	601	5	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

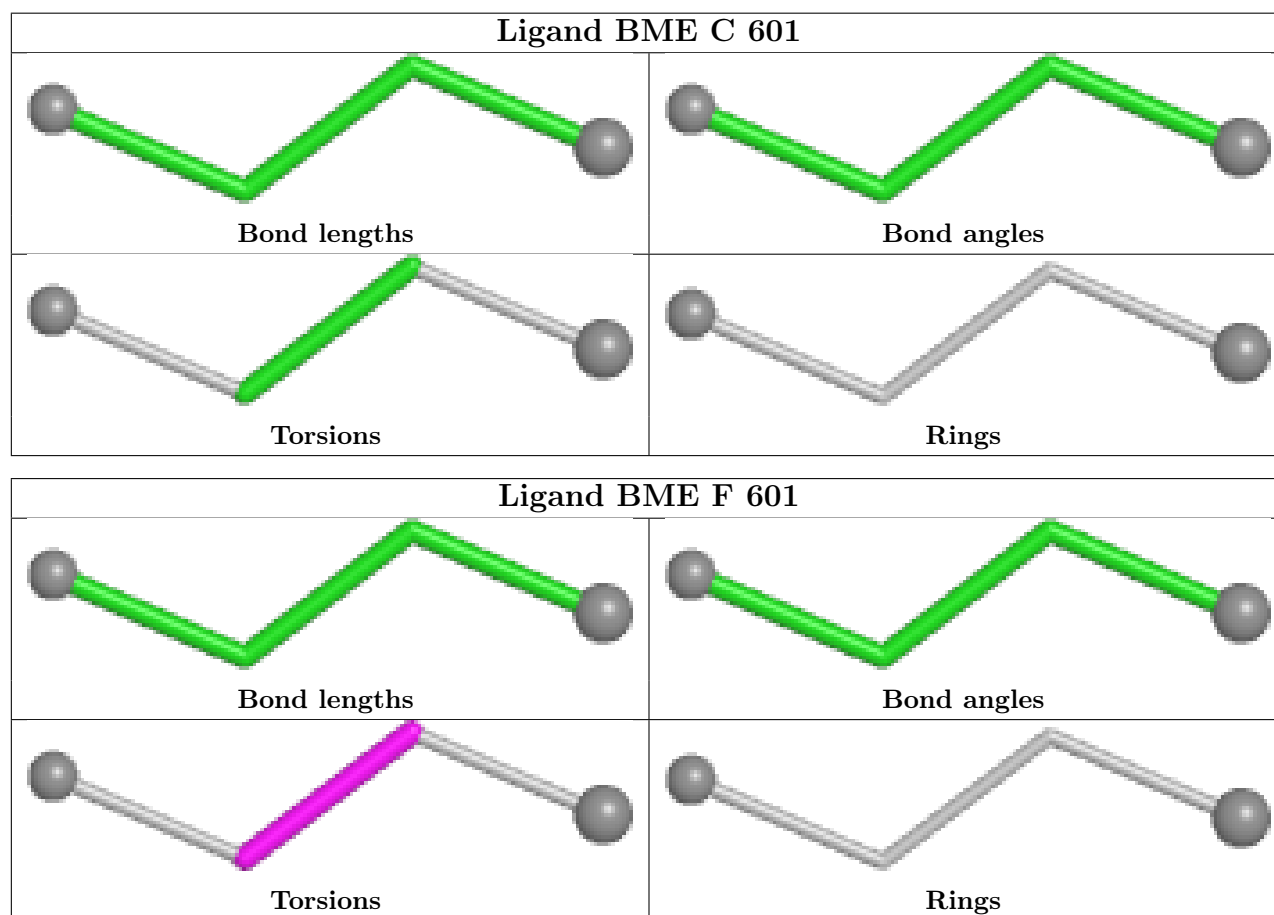
Mol	Chain	Res	Type	Atoms
4	F	601	BME	O1-C1-C2-S2

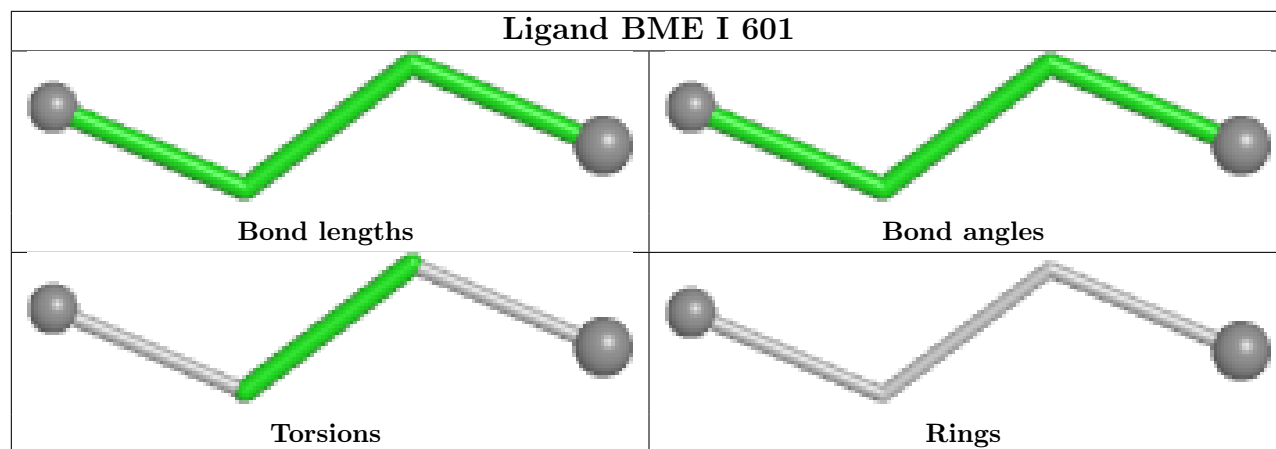
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	601	BME	1	0

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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

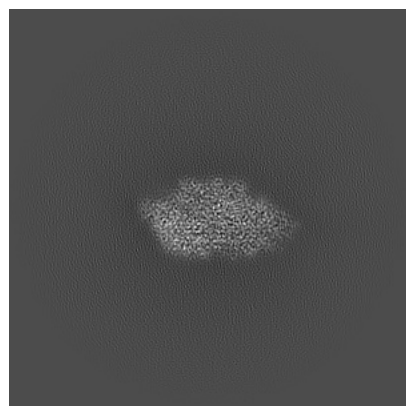
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60854. These allow visual inspection of the internal detail of the map and identification of artifacts.

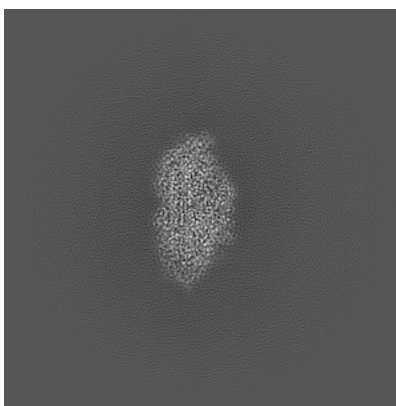
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

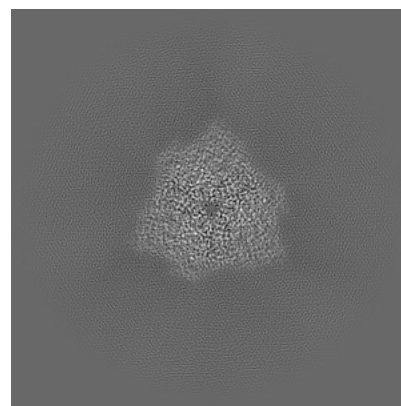
6.1.1 Primary map



X

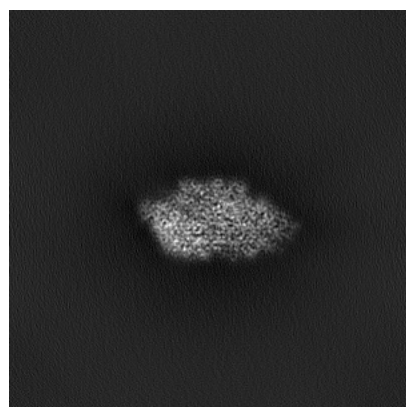


Y

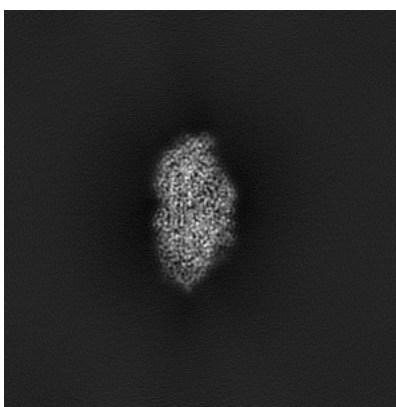


Z

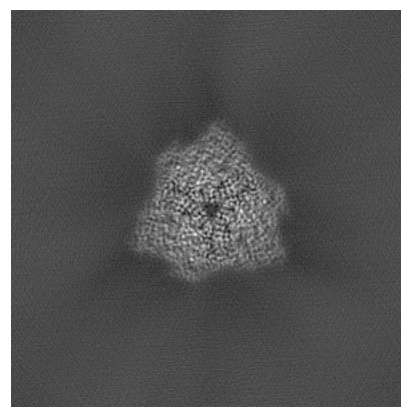
6.1.2 Raw map



X



Y

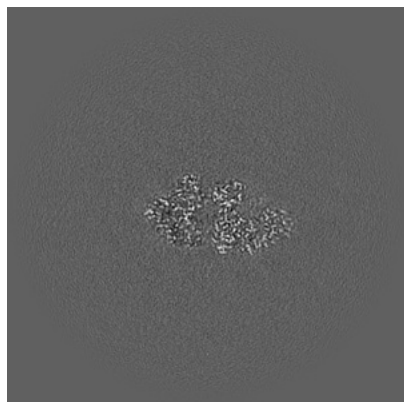


Z

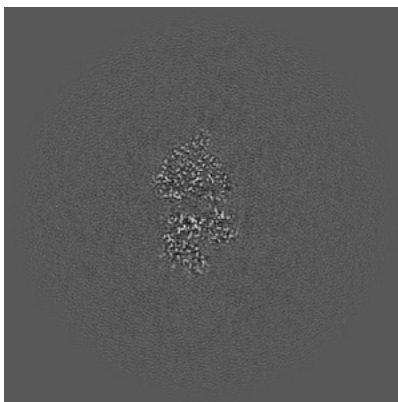
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

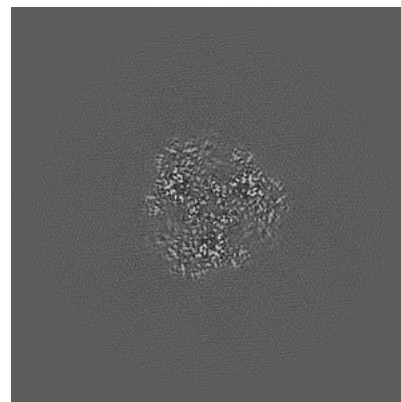
6.2.1 Primary map



X Index: 180

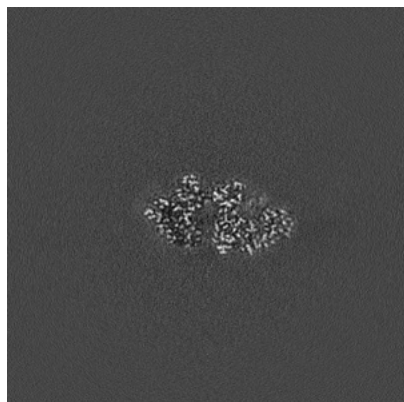


Y Index: 180

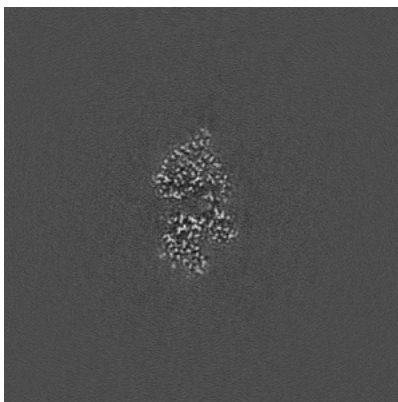


Z Index: 180

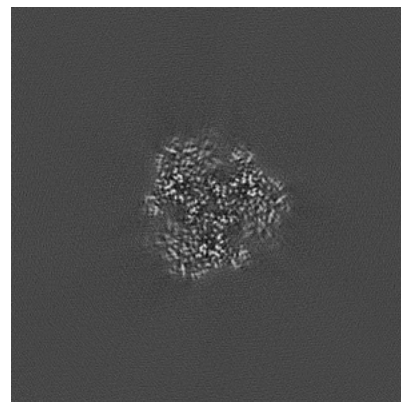
6.2.2 Raw map



X Index: 180



Y Index: 180

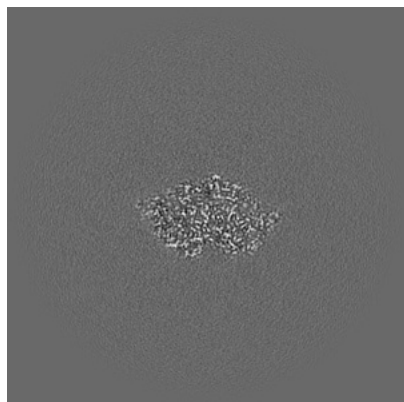


Z Index: 180

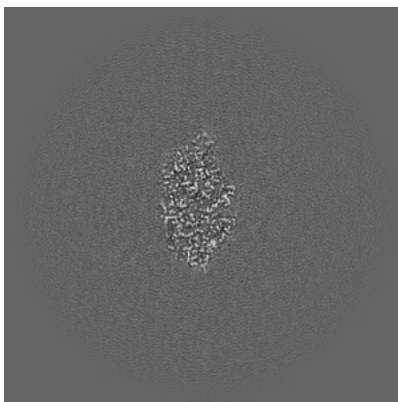
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

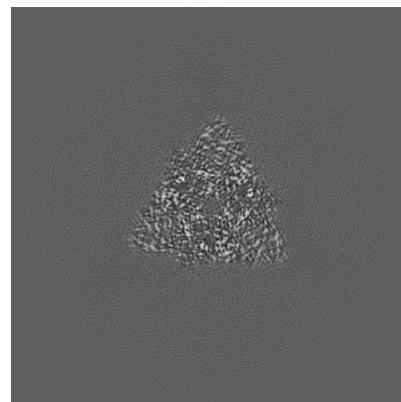
6.3.1 Primary map



X Index: 168

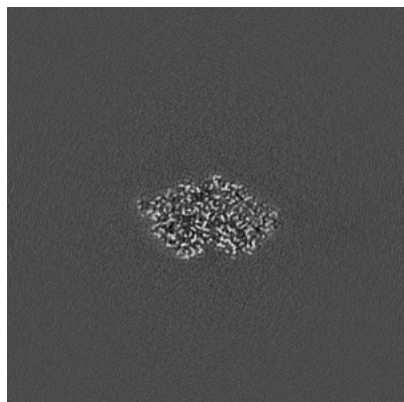


Y Index: 189

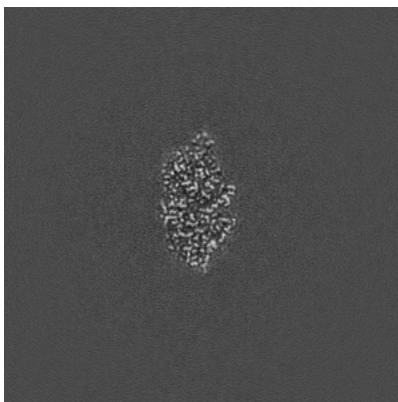


Z Index: 166

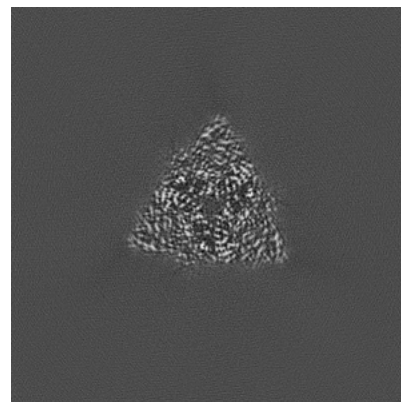
6.3.2 Raw map



X Index: 167



Y Index: 189

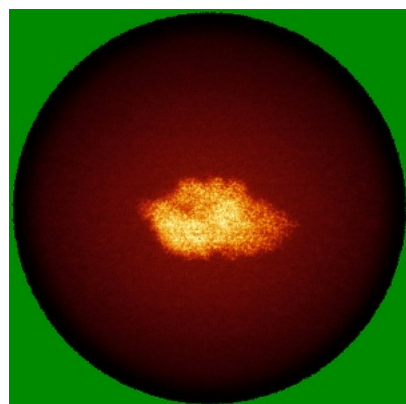


Z Index: 166

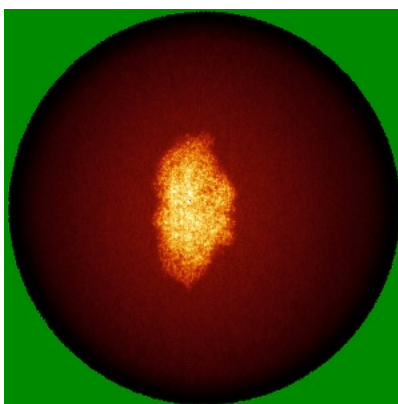
The images above show the largest variance slices of the map in three orthogonal directions.

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

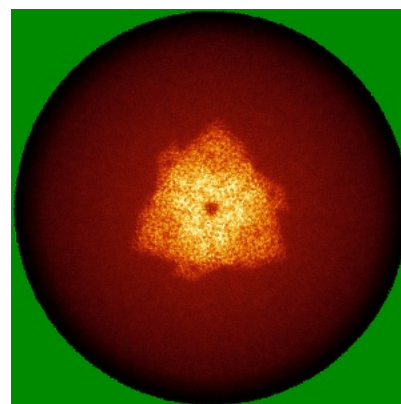
6.4.1 Primary map



X

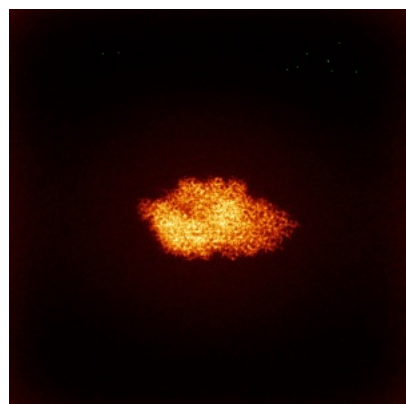


Y

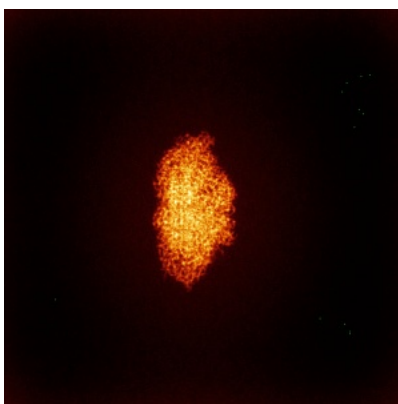


Z

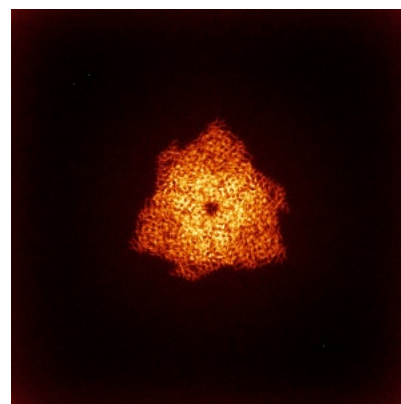
6.4.2 Raw map



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.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



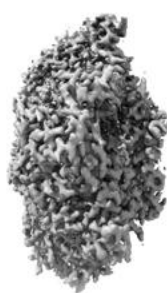
Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

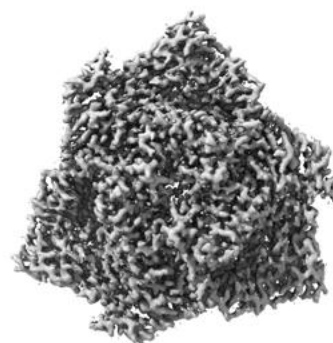
6.5.2 Raw map



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.

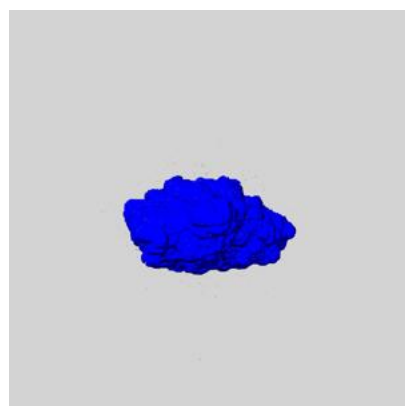
6.6 Mask visualisation [i](#)

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

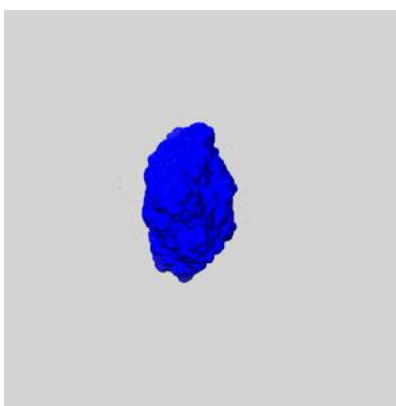
A mask typically either:

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

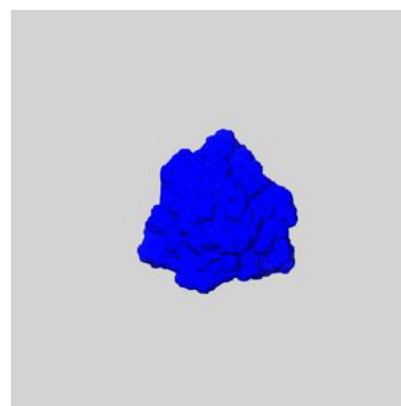
6.6.1 emd_60854_msk_1.map [i](#)



X



Y

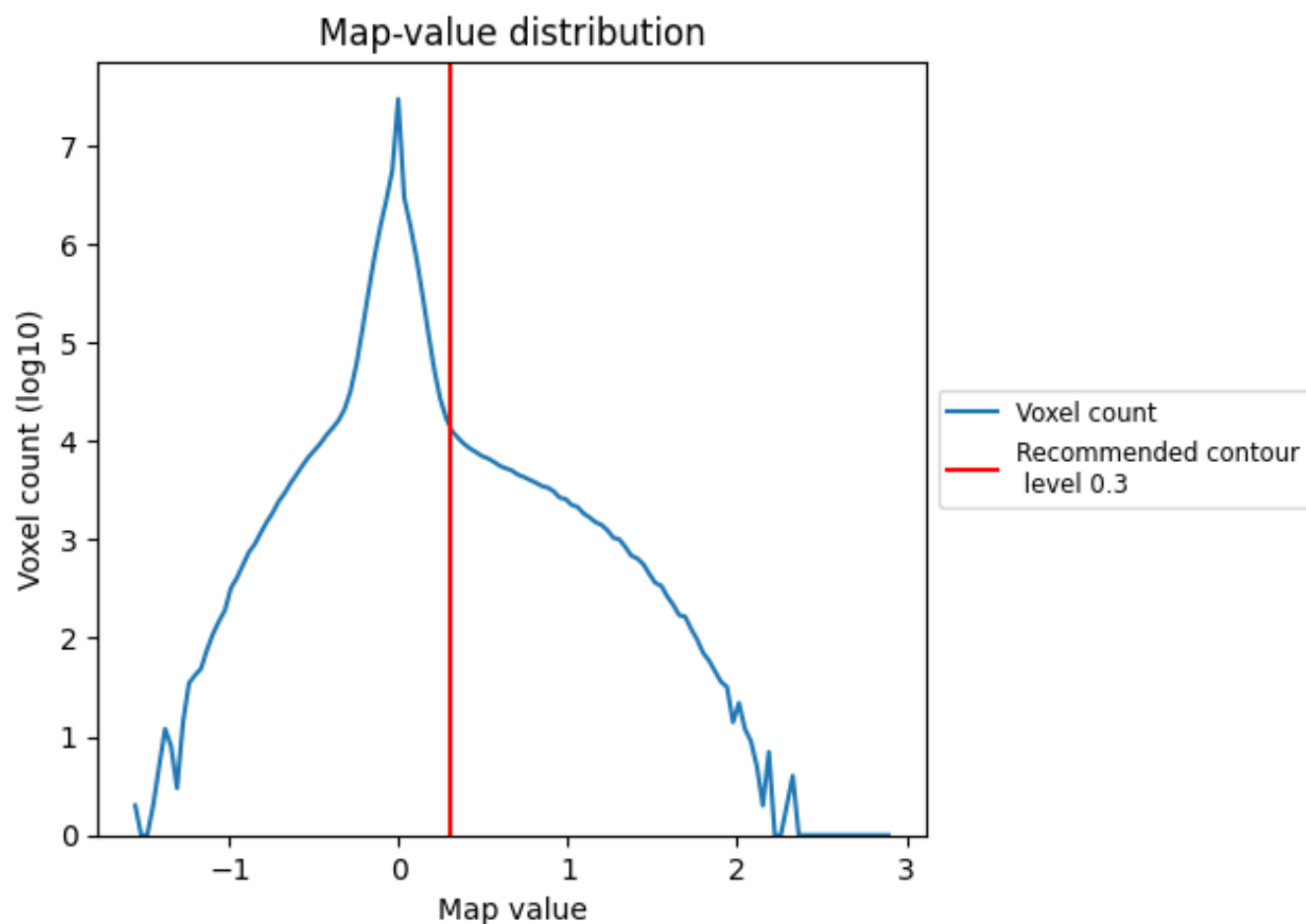


Z

7 Map analysis [i](#)

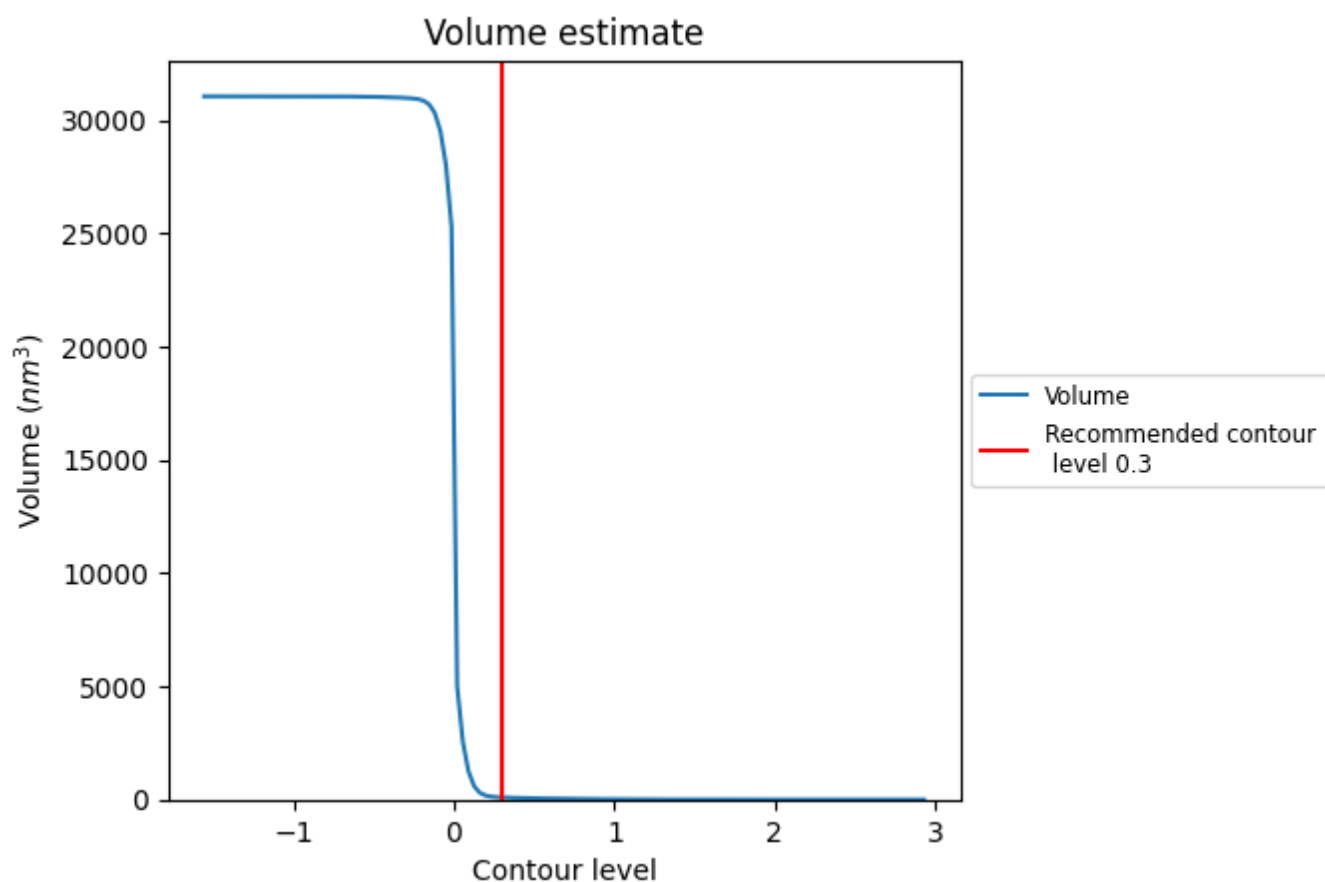
This section contains the results of statistical analysis of the map.

7.1 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.

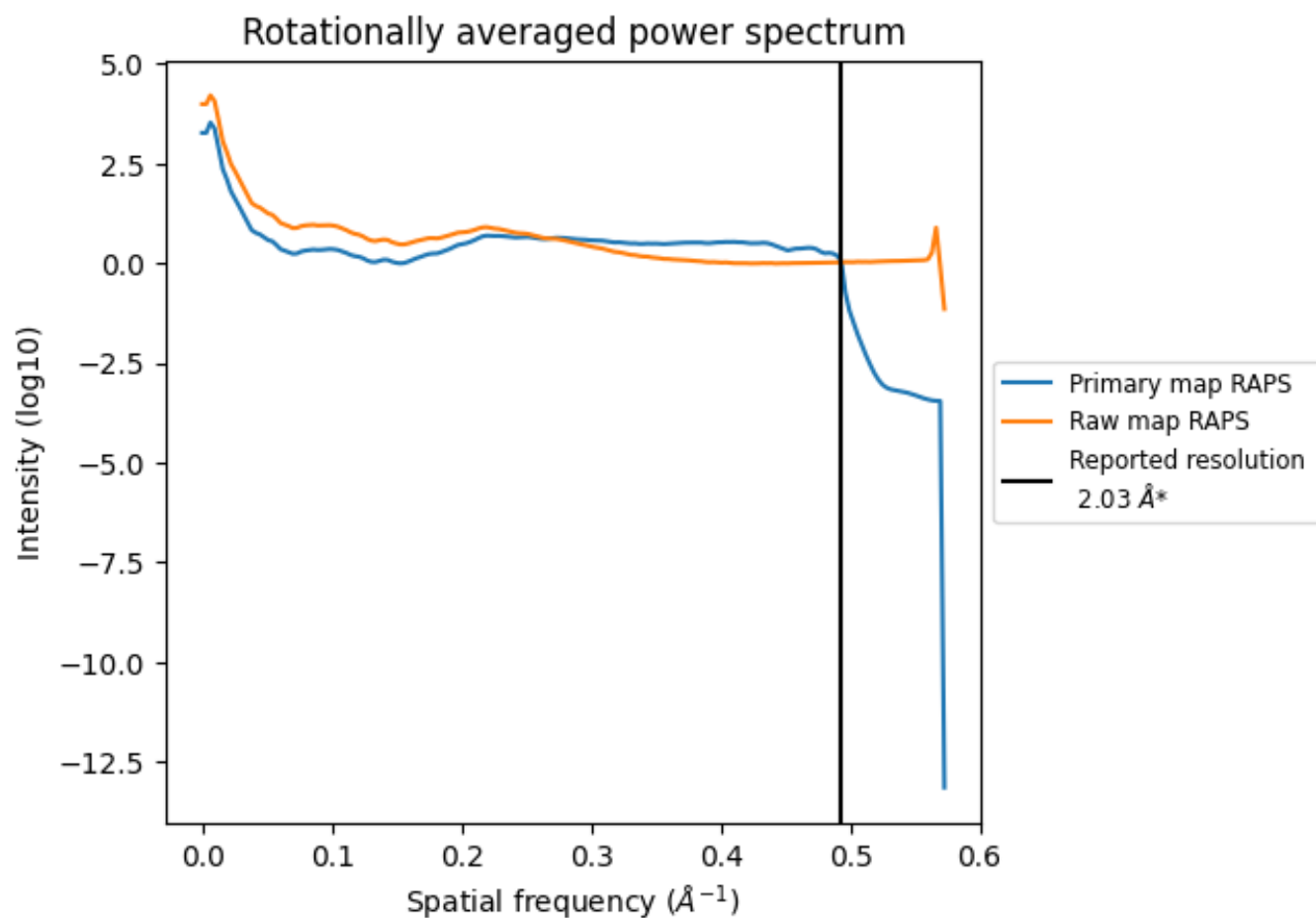
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm³; this corresponds to an approximate mass of 86 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

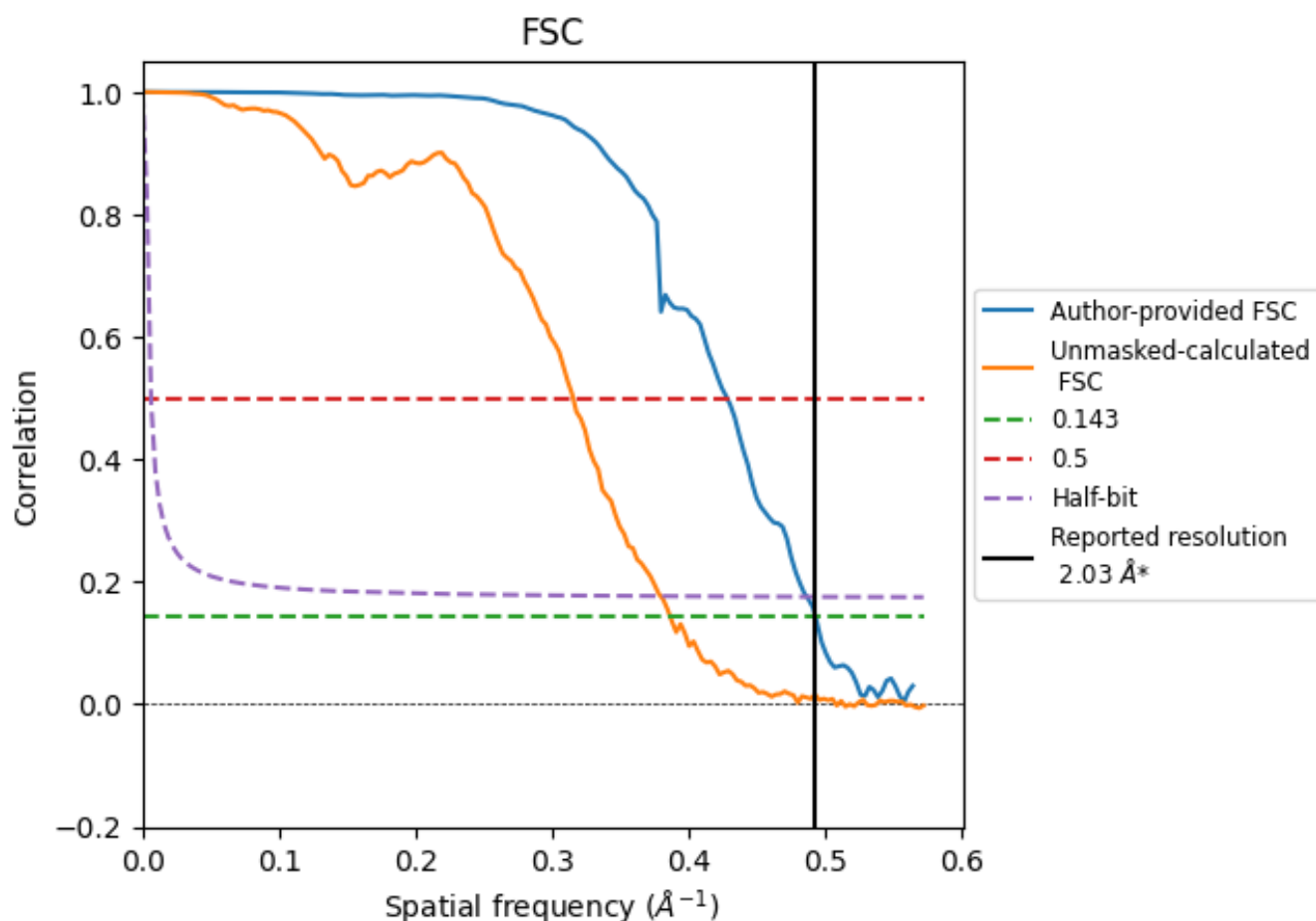


*Reported resolution corresponds to spatial frequency of 0.493 Å⁻¹

8 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.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.493 \AA^{-1}

8.2 Resolution estimates [i](#)

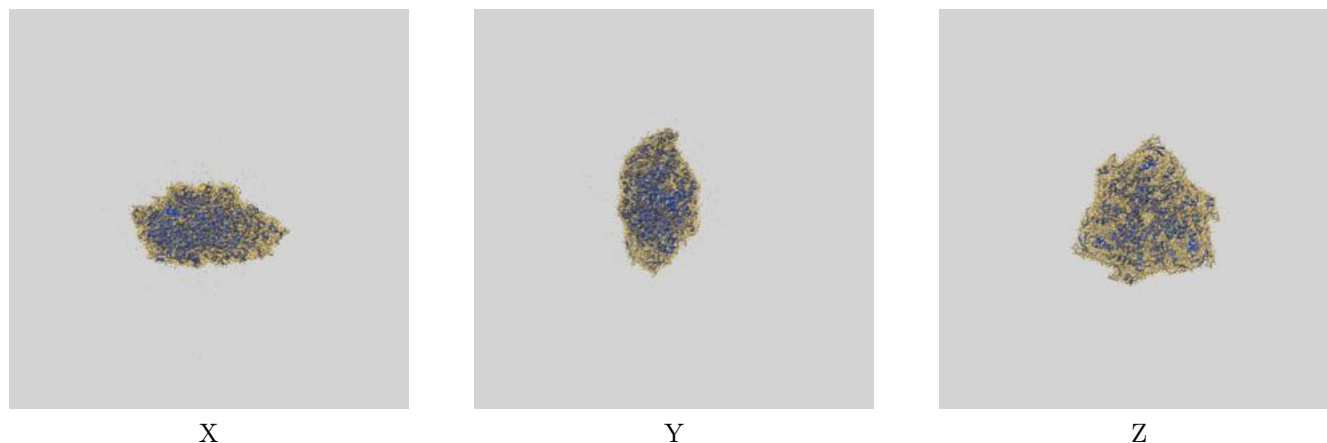
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.03	-	-
Author-provided FSC curve	2.03	2.33	2.05
Unmasked-calculated*	2.58	3.17	2.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.58 differs from the reported value 2.03 by more than 10 %

9 Map-model fit [i](#)

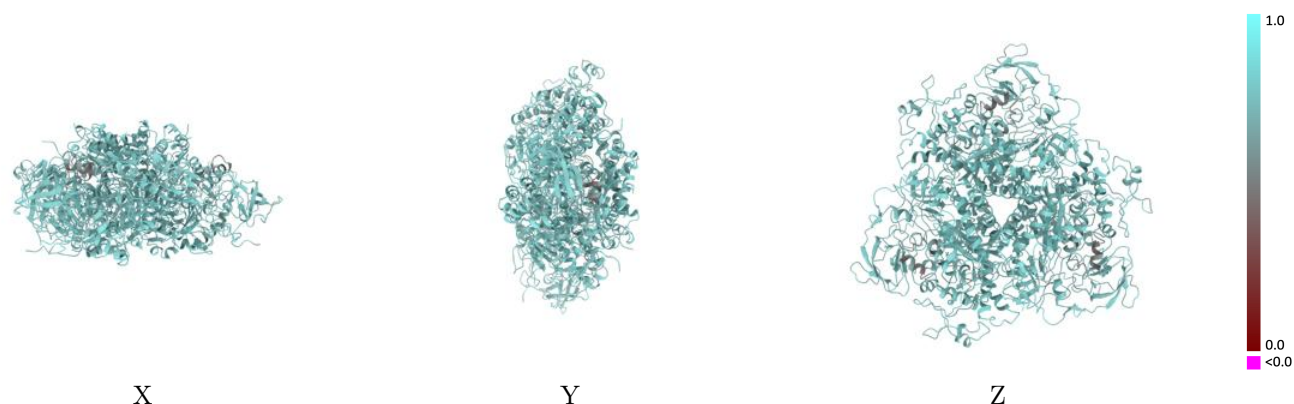
This section contains information regarding the fit between EMDB map EMD-60854 and PDB model 9IT2. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



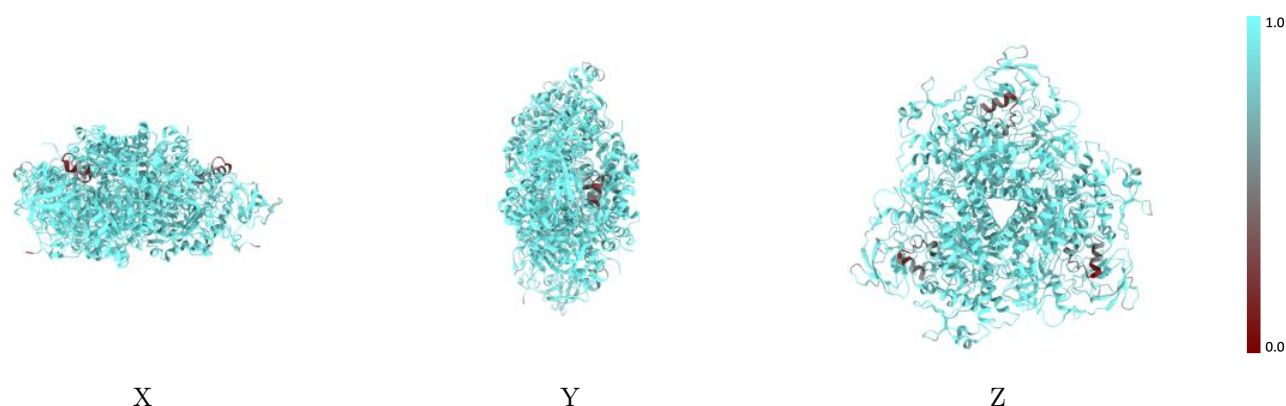
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



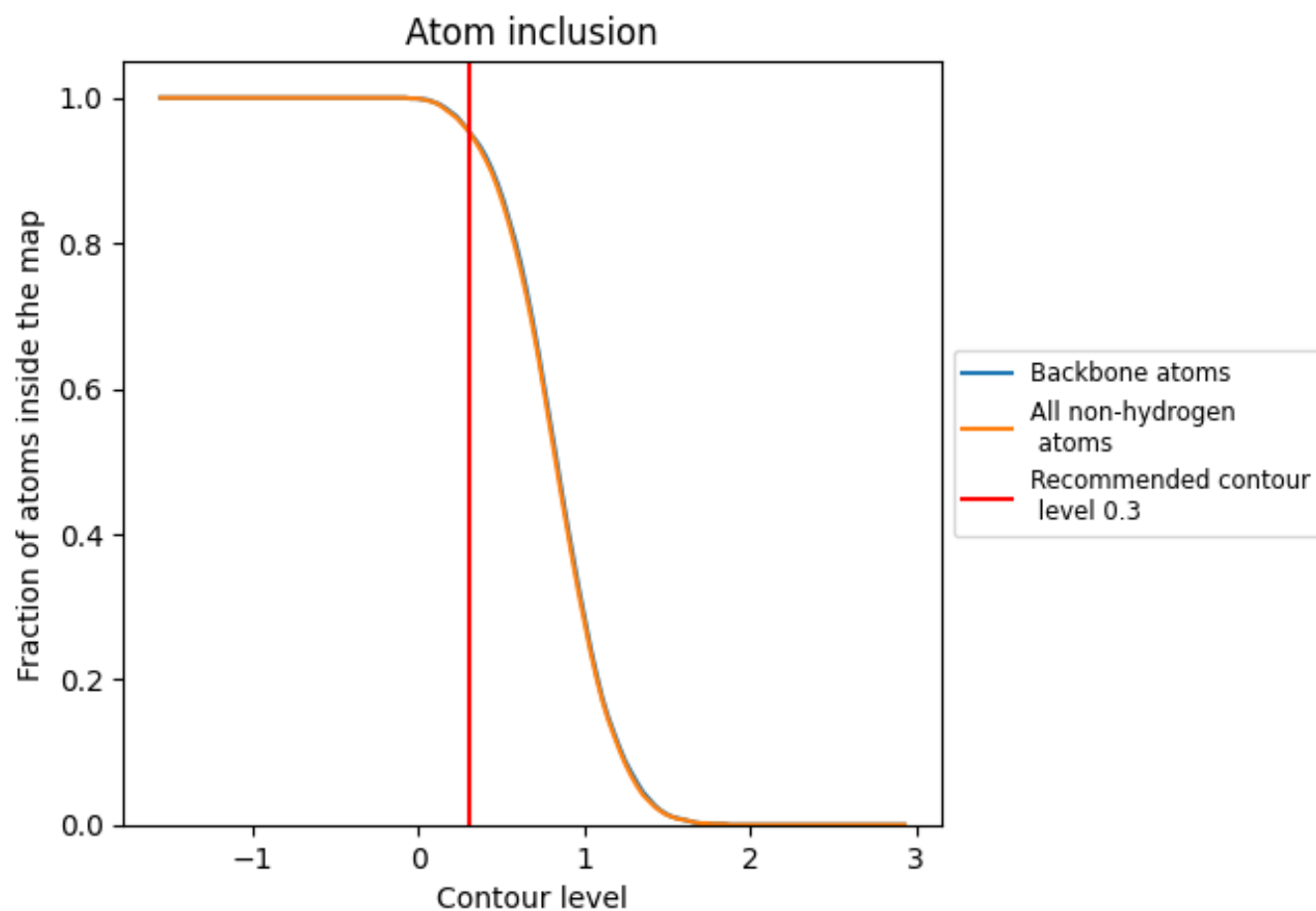
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9540	<div><div></div></div> 0.7330
A	<div><div></div></div> 0.9840	<div><div></div></div> 0.7520
B	<div><div></div></div> 0.9200	<div><div></div></div> 0.7130
C	<div><div></div></div> 0.9550	<div><div></div></div> 0.7330
D	<div><div></div></div> 0.9840	<div><div></div></div> 0.7500
E	<div><div></div></div> 0.9190	<div><div></div></div> 0.7150
F	<div><div></div></div> 0.9550	<div><div></div></div> 0.7330
G	<div><div></div></div> 0.9860	<div><div></div></div> 0.7550
H	<div><div></div></div> 0.9220	<div><div></div></div> 0.7130
I	<div><div></div></div> 0.9550	<div><div></div></div> 0.7350

1.0

0.0

<0.0