



## wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 08:24 AM EST

PDB ID : 6BCX  
EMDB ID : EMD-7087  
Title : mTORC1 structure refined to 3.0 angstroms  
Authors : Pavletich, N.P.; Yang, H.  
Deposited on : 2017-10-20  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

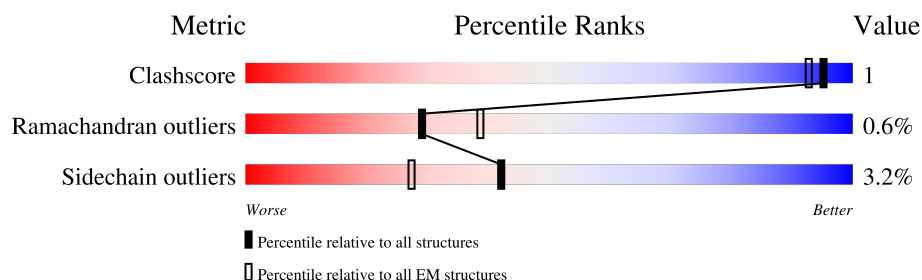
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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



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

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  $\geq 3$ , 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	2549	<div> <div>20%</div> <div>81%</div> <div>5%</div> <div>15%</div> </div>
1	B	2549	<div> <div>20%</div> <div>81%</div> <div>5%</div> <div>15%</div> </div>
2	D	326	<div> <div>42%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
2	E	326	<div> <div>39%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
3	W	1343	<div> <div>39%</div> <div>73%</div> <div>5%</div> <div>22%</div> </div>
3	Y	1343	<div> <div>39%</div> <div>74%</div> <div>.</div> <div>22%</div> </div>
4	X	122	<div> <div>6%</div> <div>.</div> <div>93%</div> </div>
4	Z	122	<div> <div>6%</div> <div>.</div> <div>93%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 113610 atoms, of which 57030 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2178	Total	C	H	N	O	S	0	0
			35034	11082	17686	3038	3117	111		
1	B	2178	Total	C	H	N	O	S	0	0
			35034	11082	17686	3038	3117	111		

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	317	Total	C	H	N	O	S	0	0
			4809	1526	2353	436	476	18		
2	E	317	Total	C	H	N	O	S	0	0
			4809	1526	2353	436	476	18		

- Molecule 3 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	W	1052	Total	C	H	N	O	S	0	0
			16791	5361	8406	1450	1518	56		
3	Y	1052	Total	C	H	N	O	S	0	0
			16791	5361	8406	1450	1518	56		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-7	MET	-	initiating methionine	UNP Q8N122
W	-6	ASP	-	expression tag	UNP Q8N122
W	-5	TYR	-	expression tag	UNP Q8N122
W	-4	LYS	-	expression tag	UNP Q8N122
W	-3	ASP	-	expression tag	UNP Q8N122
W	-2	ASP	-	expression tag	UNP Q8N122
W	-1	ASP	-	expression tag	UNP Q8N122
W	0	ASP	-	expression tag	UNP Q8N122
W	1	LYS	-	expression tag	UNP Q8N122

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-7	MET	-	initiating methionine	UNP Q8N122
Y	-6	ASP	-	expression tag	UNP Q8N122
Y	-5	TYR	-	expression tag	UNP Q8N122
Y	-4	LYS	-	expression tag	UNP Q8N122
Y	-3	ASP	-	expression tag	UNP Q8N122
Y	-2	ASP	-	expression tag	UNP Q8N122
Y	-1	ASP	-	expression tag	UNP Q8N122
Y	0	ASP	-	expression tag	UNP Q8N122
Y	1	LYS	-	expression tag	UNP Q8N122

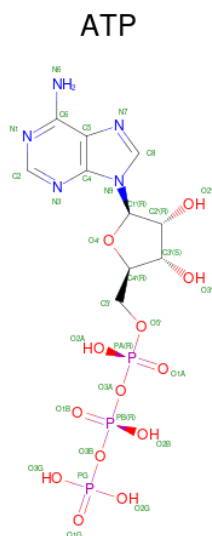
- Molecule 4 is a protein called Eukaryotic translation initiation factor 4E-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	X	8	Total	C	H	N	O	S	0	0
			126	42	58	9	16	1		
4	Z	8	Total	C	H	N	O	S	0	0
			126	42	58	9	16	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-3	GLY	-	expression tag	UNP Q13541
X	-2	SER	-	expression tag	UNP Q13541
X	-1	GLY	-	expression tag	UNP Q13541
X	0	ARG	-	expression tag	UNP Q13541
Z	-3	GLY	-	expression tag	UNP Q13541
Z	-2	SER	-	expression tag	UNP Q13541
Z	-1	GLY	-	expression tag	UNP Q13541
Z	0	ARG	-	expression tag	UNP Q13541

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

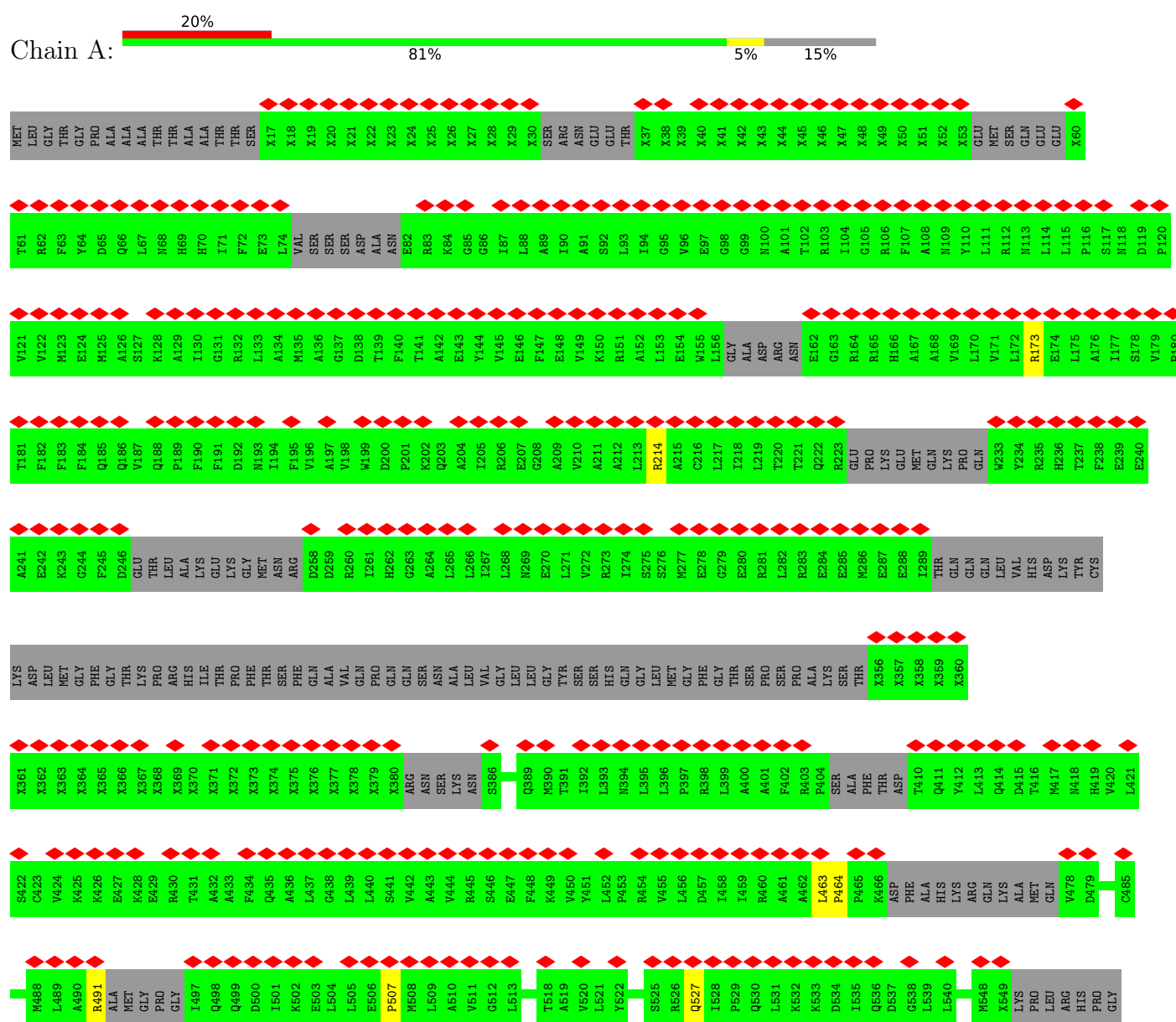
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
6	A	2	Total Mg 2 2	0
6	B	2	Total Mg 2 2	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.

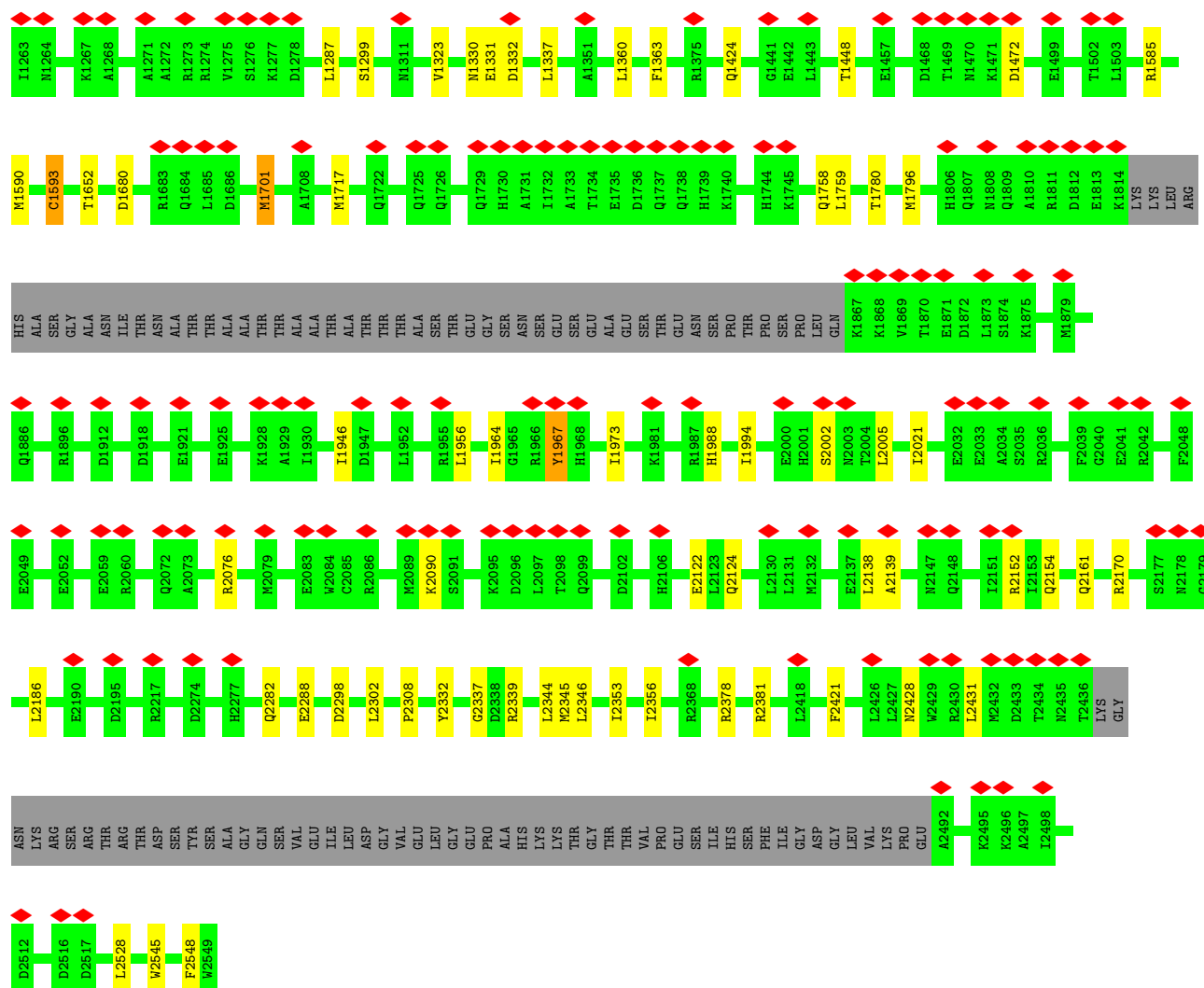
- Molecule 1: Serine/threonine-protein kinase mTOR



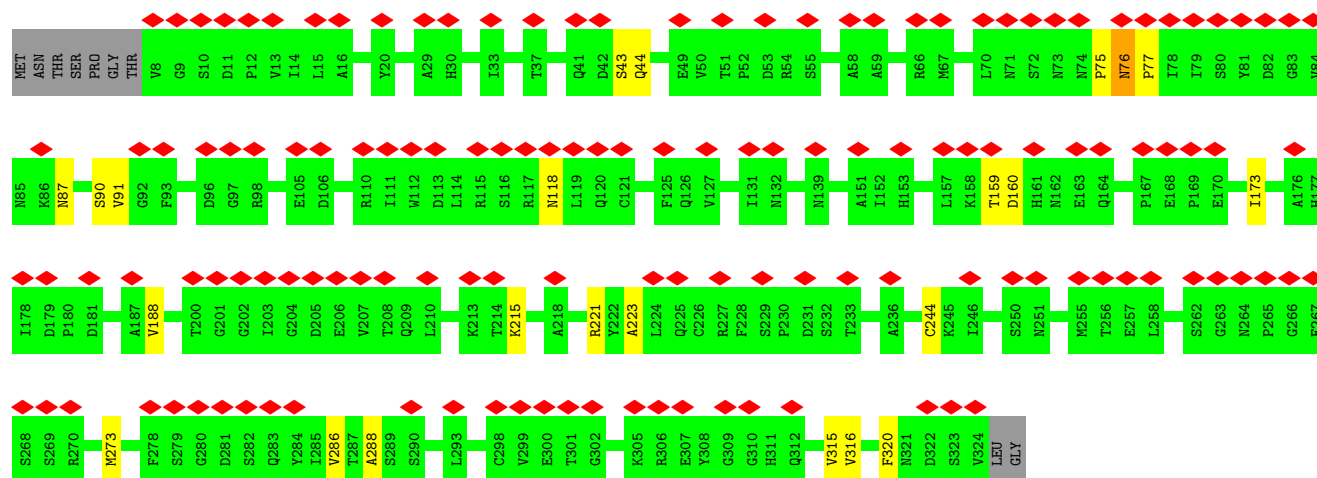
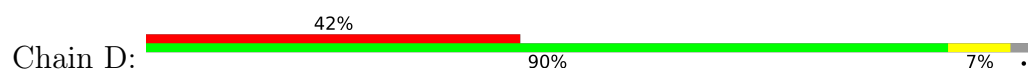


MET	LEU	GLY	THR	GLY	PRO	ALA	ALA	ALA	THR	THR	ALA	ALA	THR	SER	X17	X18	X19	X20	X21	X22	X23	X24	X25	X26	X27	X28	X29	X30	SER	ARG	ASN	GLU	GLU	THR	X37	X38	X39	X40	X41	X42	X43	X44	X45	X46	X47	X48	X49	X50	X51	X52	X53	MET	SER	GLN	GLU	GLU	X60				
T61	R62	F63	F63	Y64	D65	Q66	L67	M68	H69	H70	I71	F72	E73	L74	VAL	SER	SER	SER	SER	ASP	ALA	ASN	E82	R83	K84	G85	G86	I87	L88	A89	I90	A91	S92	L93	I94	G95	V96	E97	G98	G99	N100	A101	T102	R103	I104	G105	R106	F107	A108	N109	Y110	L111	R112	M113	L114	L115	P116	S117	M118	D119	P120
V121	V122	M123	E124	M125	A126	S127	A128	A129	I130	G131	R132	L133	A134	M135	A136	G137	D138	T139	F140	T141	A142	E143	Y144	V145	E146	F147	E148	V149	K150	R151	A152	L153	E154	W155	L156	GLY	ALA	ASP	ARG	ASN	E162	G163	R164	R165	H166	A167	A168	V169	L170	V171	L172	R173	E174	L175	A176	S177	M178	V179	P180		
T181	F182	F183	F184	Q185	Q186	V187	Q188	F189	F190	F191	D192	M193	I194	F195	V196	A197	V198	W199	D200	P201	K202	Q203	A204	I205	R206	E207	G208	A209	V210	A211	A212	L213	R214	A215	C216	L217	I218	I219	L220	T221	Q222	R223	GLU	PRO	LYS	GLU	GLN	LYS	PRO	GLN	W233	Y234	R235	H236	T237	F238	E239	E240			
A241	E242	K243	G244	F245	D246	GLU	THR	LEU	ALA	LYS	GLU	GLY	MET	ASN	ARG	D258	D259	R260	I261	H262	G263	A264	L265	L266	I267	L268	N269	E270	L271	V272	R273	L274	S275	S276	M277	E278	G279	E280	R281	L282	E284	E285	M286	E287	E288	I289	THR	GLN	GLN	LEU	VAL	HIS	ASP	LYS	CYS						
LYS	ASP	LEU	MET	PHE	GLY	THR	LYS	PRO	ARG	HIS	ILE	THR	PHE	THR	PHE	GLN	ALA	VAL	GLN	PRO	GLN	ASN	ALA	LEU	GLY	LEU	GLY	TYR	SER	SER	HIS	GLN	GLY	LEU	MET	PHE	GLY	THR	THR	ALA	THR	X356	X357	X358	X359	X360															
X361	X362	X363	X364	X367	X368	X369	X370	X371	X372	X373	X374	X375	X376	X377	X378	X379	X380	ARG	ASN	LYS	ASN	S386	L387	I388	Q389	M390	T391	I392	L393	N394	L395	L396	P397	R398	L399	A400	A401	F402	R403	P404	SER	ALA	PHE	THR	ASP	T410	Q411	Y412	L413	Q414	D415	T416	M417	N418	H419	V420	L421				
S422	C423	V424	K425	K426	E427	K428	R429	R430	T431	A432	A433	F434	Q435	A436	L437	G438	L439	L440	S441	V442	A443	V444	R445	S446	E447	F448	K449	V450	Y451	L452	L453	R454	V455	L456	D457	I458	I459	R460	A461	A462	L463	P464	P465	K466	ASP	PHE	ALA	HIS	LYS	ARG	GLN	LYS	ALA	MET	GLN	V478	D479	F483			
T484	C485	L489	A490	R491	ALA	MET	GLY	PRO	GLY	I497	Q498	Q499	D500	I501	K502	E503	L504	L505	E506	P507	M508	L509	A510	V511	G512	L513	T518	Y522	D523	L524	S525	R526	Q527	I528	P529	Q530	L531	K532	K533	D534	I535	G538	X549	LYS	PRO	LEU	ARG	HIS	PRO	GLY	MET	PRO	LYS	GLY							
LEU	ALA	HIS	GLN	LEU	ALA	SER	PRO	GLY	THR	THR	LEU	PRO	GLU	ALA	SER	X578	V579	L584	S591	F592	E595	GLY	HIS	S599	F602	L611	N612	A623	L630	T631	P632	S633	ILE	HIS	LEU	ILE	SER	GLY	HIS	ALA	HIS	VAL	V644	S645	Q646	V652	L656														
V675	R755	L760	L767	P786	ASP	PRO	ASP	PRO	N791	V794	N797	S809	F821	Q829	D830	S831	S832	L833	L834	T851	V854	V855	R859	T863	V867	N870	Q876	R882	A893	L894	I903	GLY	MET	ILE	ASP	GLN	SER	ARG	ASP	ALA																					
SER	ALA	VAL	SER	LEU	SER	GLU	SER	LYS	ASP	GLN	ASP	SER	SER	TYR	SER	THR	SER	E933	M934	N937	D961	Q962	S965	H968	D1005	G1006	Q1014	L1019	M1044	L1055	V1081	H1084	D1085	M1086	S1087	I1091	L1102	L1121	F1122	D1123	E1126																				
I1155	I1159	V1160	R1161	D1164	E1168	S1179	Q1183	V1198	I1213	T1221	L1222	ALA	ASP	GLU	GLU	ASP	PRO	LEU	ILE	TYR	GLN	HIS	ARG	MET	ARG	GLY	GLN	ASP	ALA	LEU	ALA	SER	GLY	PRO	MET	LYS	LEU	HIS	VAL	S1261	T1262																				



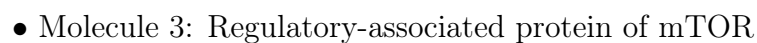


- Molecule 2: Target of rapamycin complex subunit LST8



- Molecule 2: Target of rapamycin complex subunit LST8

Response	Percentage
Yes	39%
No	90%
Don't know	7%



Response	Percentage
Good job	39%
Not doing a good job	61%
Not doing a good job at all	5%
Not doing a good job	56%







Chain Z:  6% 93%

GLY	SER	GLY	ARG	MET	SER	GLY	GLY	SER	SER	CYS	SER	GLN	THR	PRO	SER	SER	ARG	ALA	ILE	PRO	ALA	THR	ARG	ARG	VAL	VAL	LEU	GLY	ASP	GLY	VAL	GLN	LEU	PRO	PRO	GLY	ASP	TYR	THR	THR	THR	PRO	GLY	GLY	THR	LEU	PHE	SER	THR	THR	PRO	GLY	GLY	THR	ARG	ILE	ILE	TYR	ASP	ARG
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LYS	PHE	LEU	MET	GLU	CYS	ARG	ASN	SER	PRO	VAL	THR	LYS	THR	PRO	PRO	ASP	LEU	PRO	THR	ILE	PRO	GLY	VAL	THR	SER	PRO	SER	SER	ASP	GLU	PRO	PRO	MET	GLU	ALA	SER	GLN	SER	HIS	LEU	ARG	ASN	SER	PRO	GLU	ASP	LYS	ARG	ALA	GLY	GLY	GLU	GLU	E111	D117	I118
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	580768	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 ( $e^-/\text{\AA}^2$ )	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.282	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	497.6444, 497.6444, 497.6444	wwPDB
Map dimensions	374, 374, 374	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3306, 1.3306, 1.3306	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: ATP, MG

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	0.42	0/17398	0.63	1/23547 (0.0%)
1	B	0.42	0/17398	0.62	1/23547 (0.0%)
2	D	0.39	0/2514	0.59	0/3426
2	E	0.39	0/2514	0.60	0/3426
3	W	0.41	0/8585	0.63	0/11680
3	Y	0.41	0/8585	0.63	0/11680
4	X	0.50	0/68	0.58	0/89
4	Z	0.51	0/68	0.58	0/89
All	All	0.41	0/57130	0.62	2/77484 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1055	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	1055	LEU	CA-CB-CG	5.43	127.79	115.30

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	17348	17686	17376	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	17348	17686	17376	34	0
2	D	2456	2353	2341	9	0
2	E	2456	2353	2341	9	0
3	W	8385	8406	8375	18	0
3	Y	8385	8406	8375	15	0
4	X	68	58	57	0	0
4	Z	68	58	57	0	0
5	A	31	12	12	0	0
5	B	31	12	12	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
All	All	56580	57030	56322	113	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 1.

The worst 5 of 113 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)
1:A:2378:ARG:NH2	1:A:2545:TRP:O	2.18	0.77
1:B:2378:ARG:NH2	1:B:2545:TRP:O	2.18	0.77
3:Y:426:ASN:N	3:Y:426:ASN:HD22	1.96	0.63
3:W:426:ASN:HD22	3:W:426:ASN:N	1.96	0.60
1:B:755:ARG:HB2	1:B:797:ASN:HD22	1.68	0.58

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2088/2549 (82%)	1972 (94%)	107 (5%)	9 (0%)	34 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	2088/2549 (82%)	1973 (94%)	106 (5%)	9 (0%)	34 72
2	D	315/326 (97%)	279 (89%)	32 (10%)	4 (1%)	12 45
2	E	315/326 (97%)	279 (89%)	32 (10%)	4 (1%)	12 45
3	W	1040/1343 (77%)	948 (91%)	85 (8%)	7 (1%)	22 60
3	Y	1040/1343 (77%)	948 (91%)	85 (8%)	7 (1%)	22 60
4	X	6/122 (5%)	6 (100%)	0	0	100 100
4	Z	6/122 (5%)	5 (83%)	1 (17%)	0	100 100
All	All	6898/8680 (80%)	6410 (93%)	448 (6%)	40 (1%)	29 64

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	893	ALA
3	W	53	ASP
1	B	893	ALA
3	Y	53	ASP
1	A	1006	GLY

### 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	1861/2166 (86%)	1803 (97%)	58 (3%)	40 75
1	B	1861/2166 (86%)	1804 (97%)	57 (3%)	40 75
2	D	269/276 (98%)	263 (98%)	6 (2%)	52 81
2	E	269/276 (98%)	263 (98%)	6 (2%)	52 81
3	W	928/1171 (79%)	895 (96%)	33 (4%)	35 70
3	Y	928/1171 (79%)	895 (96%)	33 (4%)	35 70
4	X	8/104 (8%)	7 (88%)	1 (12%)	4 20
4	Z	8/104 (8%)	7 (88%)	1 (12%)	4 20
All	All	6132/7434 (82%)	5937 (97%)	195 (3%)	42 74

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1055	LEU
1	B	2138	LEU
1	B	1126	GLU
1	B	1593	CYS
1	B	2346	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2124	GLN
3	Y	412	GLN
1	B	2154	GLN
2	E	321	ASN
3	Y	995	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are 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
5	ATP	A	3000	6	26,33,33	1.01	2 (7%)	31,52,52	1.38	5 (16%)
5	ATP	B	3000	6	26,33,33	1.05	1 (3%)	31,52,52	1.46	6 (19%)

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
5	ATP	A	3000	6	-	2/18/38/38	0/3/3/3
5	ATP	B	3000	6	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	3000	ATP	C5-C4	2.68	1.48	1.40
5	A	3000	ATP	C5-C4	2.48	1.47	1.40
5	A	3000	ATP	O4'-C1'	2.01	1.43	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3000	ATP	N3-C2-N1	-3.83	122.70	128.68
5	A	3000	ATP	N3-C2-N1	-3.80	122.73	128.68
5	B	3000	ATP	C4-C5-N7	-2.98	106.29	109.40
5	A	3000	ATP	C4-C5-N7	-2.81	106.47	109.40
5	B	3000	ATP	C3'-C2'-C1'	2.47	104.70	100.98

There are no chirality outliers.

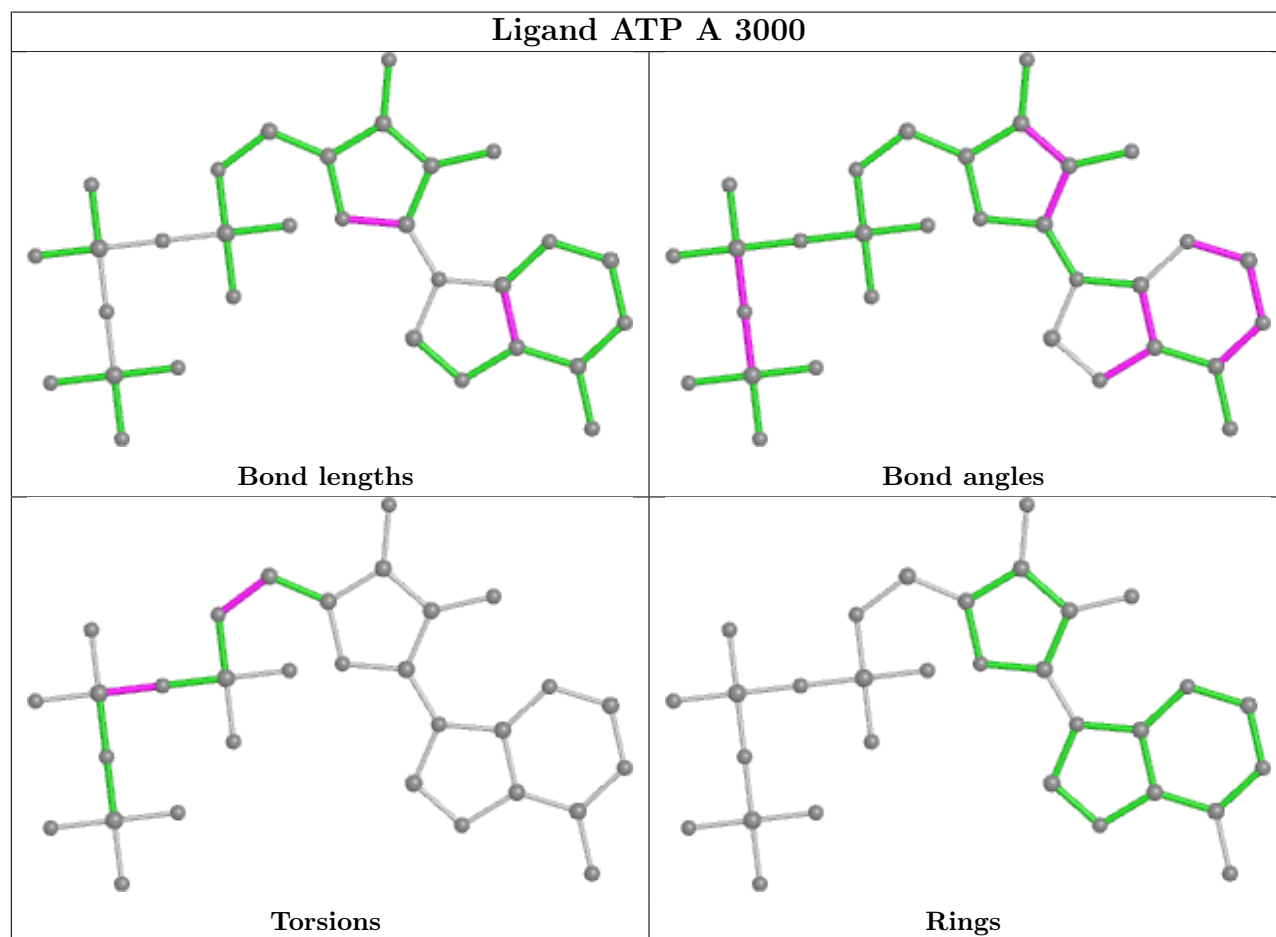
5 of 6 torsion outliers are listed below:

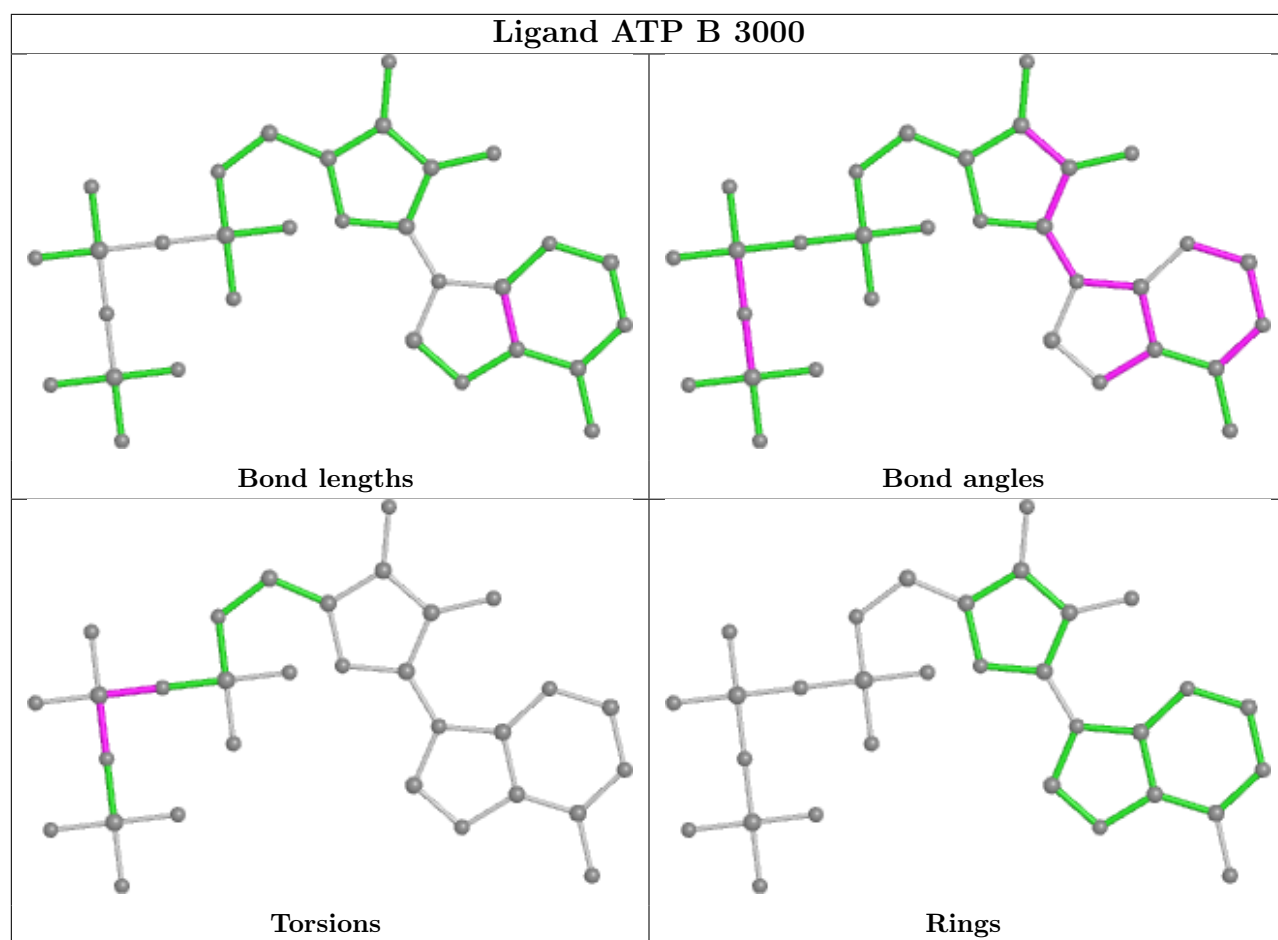
Mol	Chain	Res	Type	Atoms
5	B	3000	ATP	PG-O3B-PB-O1B
5	B	3000	ATP	PA-O3A-PB-O1B
5	A	3000	ATP	PA-O3A-PB-O2B
5	B	3000	ATP	PA-O3A-PB-O2B
5	A	3000	ATP	C4'-C5'-O5'-PA

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.





## 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.

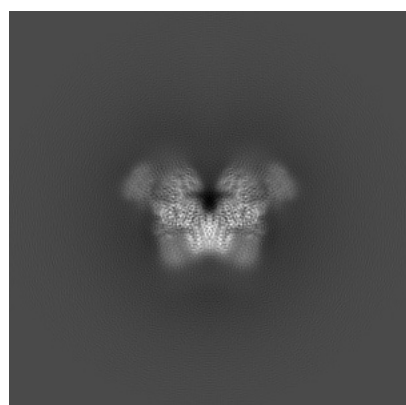
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7087. These allow visual inspection of the internal detail of the map and identification of artifacts.

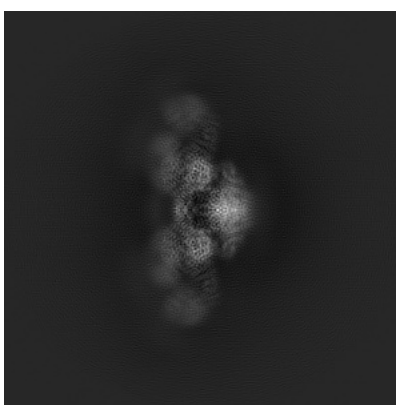
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

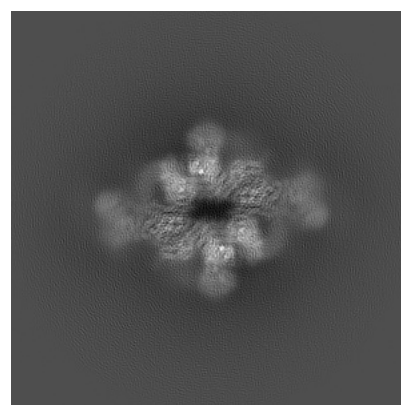
#### 6.1.1 Primary map



X



Y

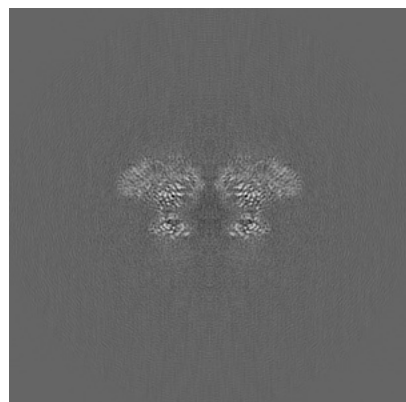


Z

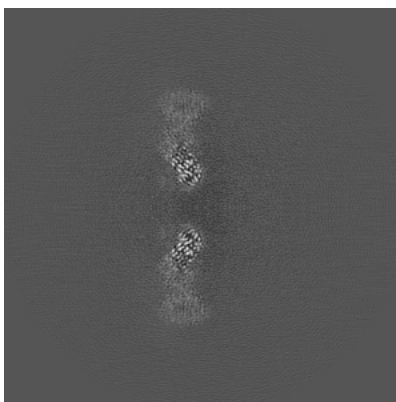
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

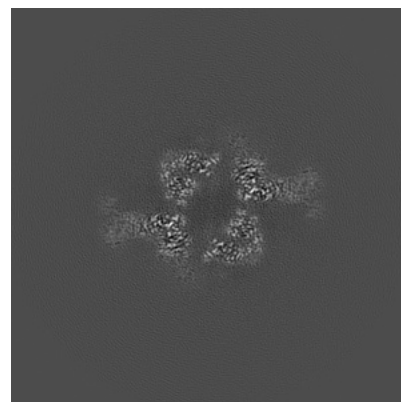
#### 6.2.1 Primary map



X Index: 187



Y Index: 187

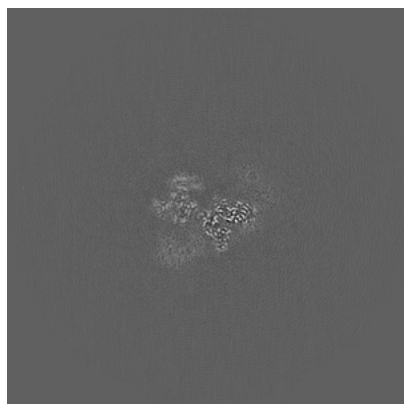


Z Index: 187

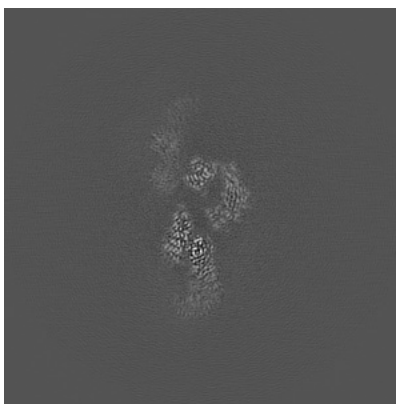
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

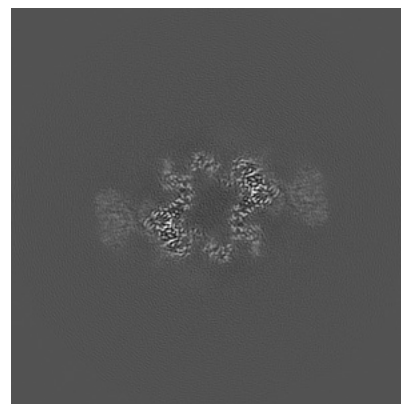
### 6.3.1 Primary map



X Index: 222



Y Index: 169

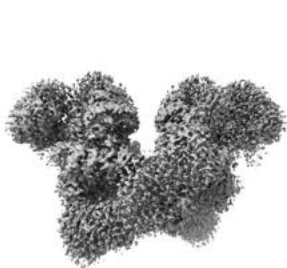


Z Index: 177

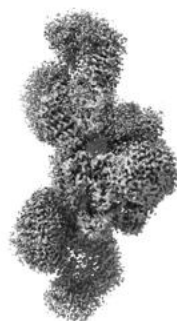
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

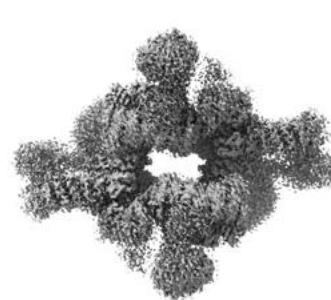
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Mask visualisation

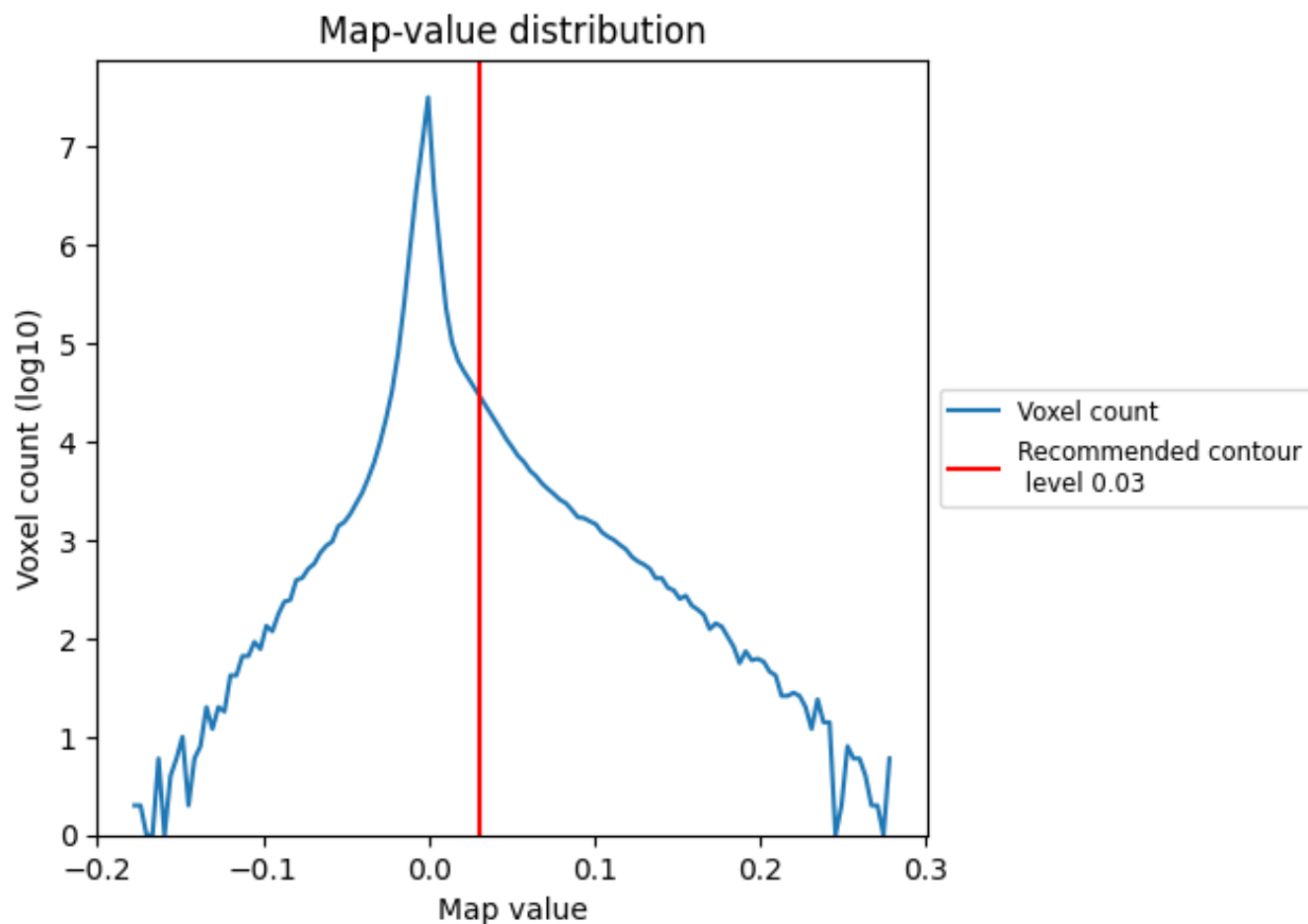
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

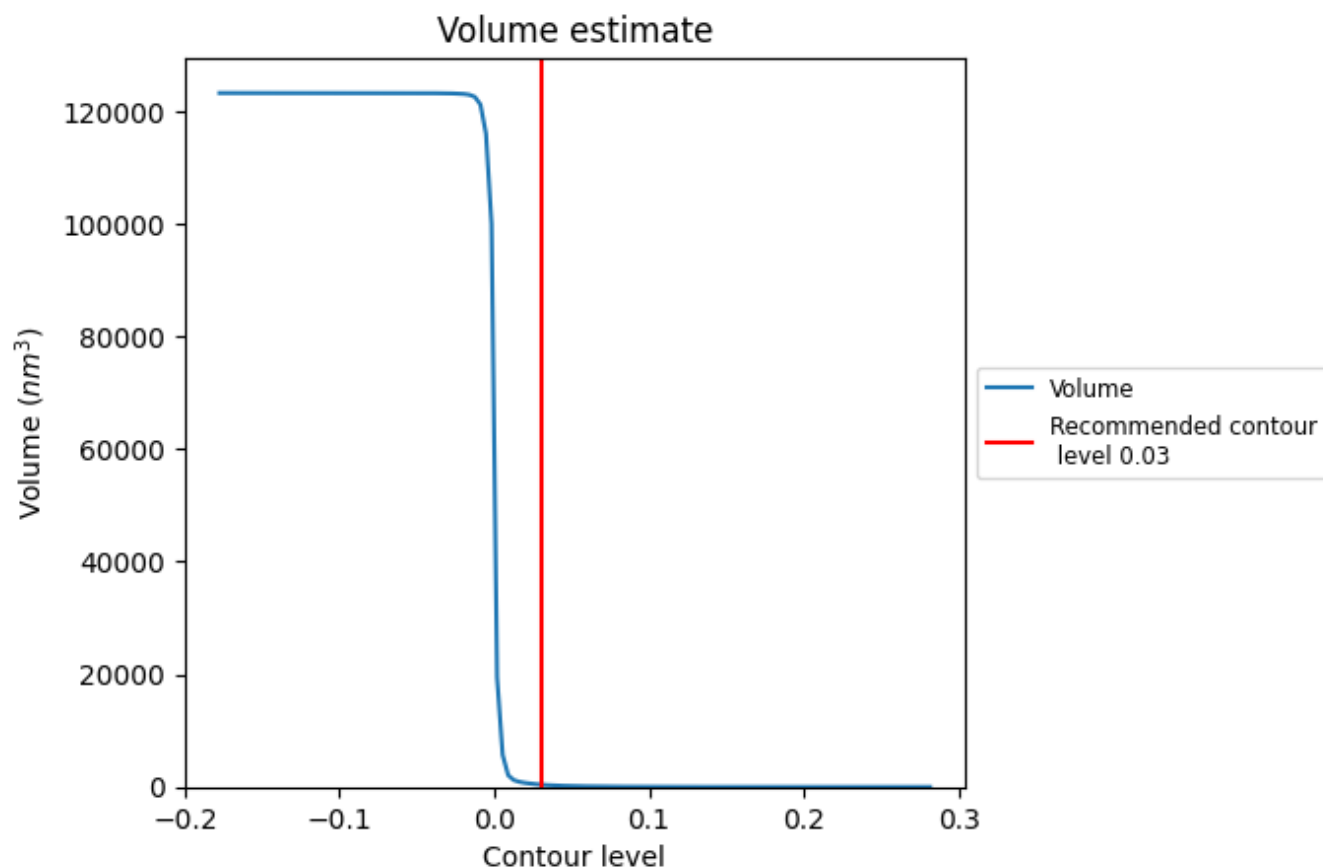
This section contains the results of statistical analysis of the map.

### 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.

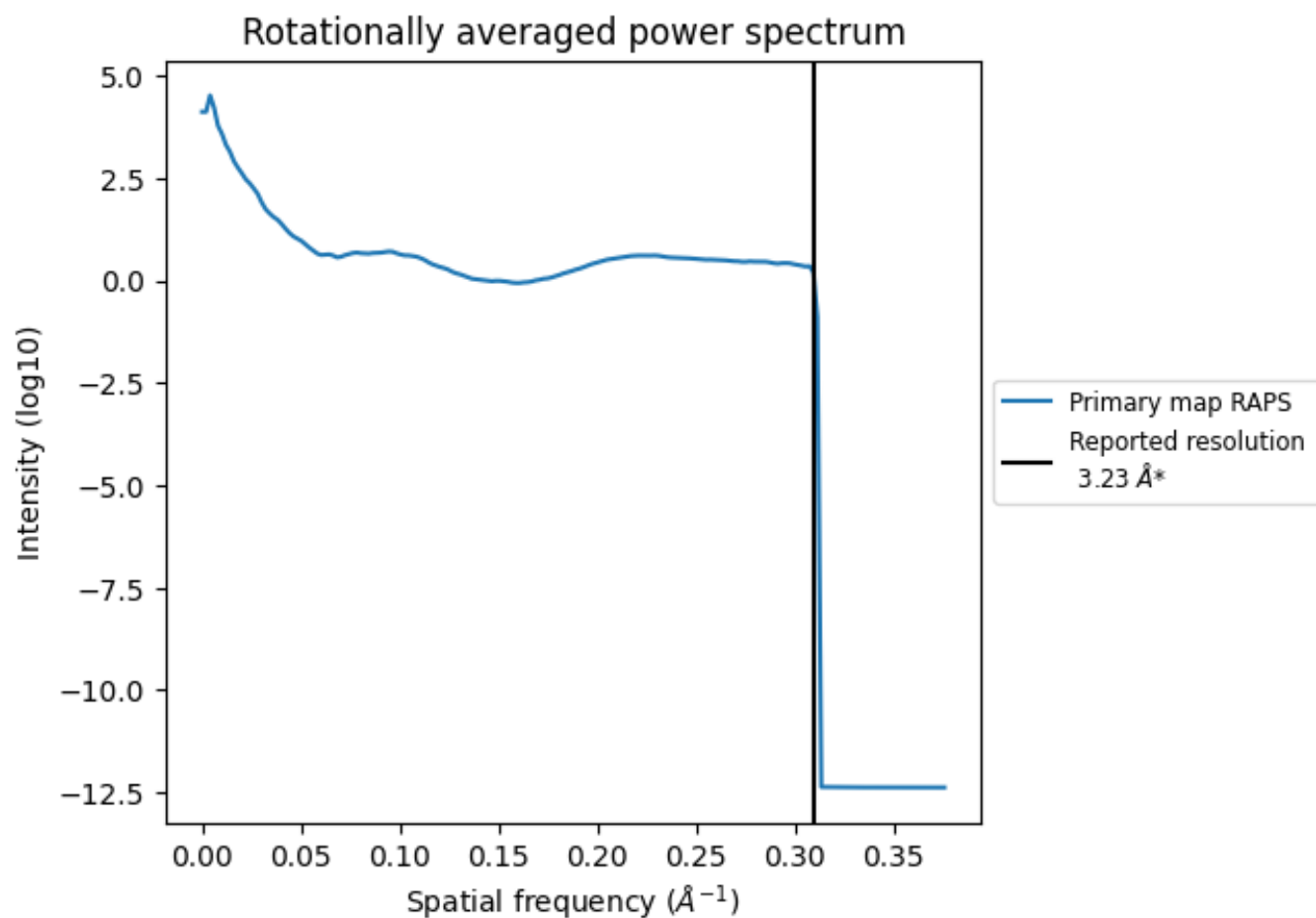
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm<sup>3</sup>; this corresponds to an approximate mass of 372 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 0.310 Å<sup>-1</sup>

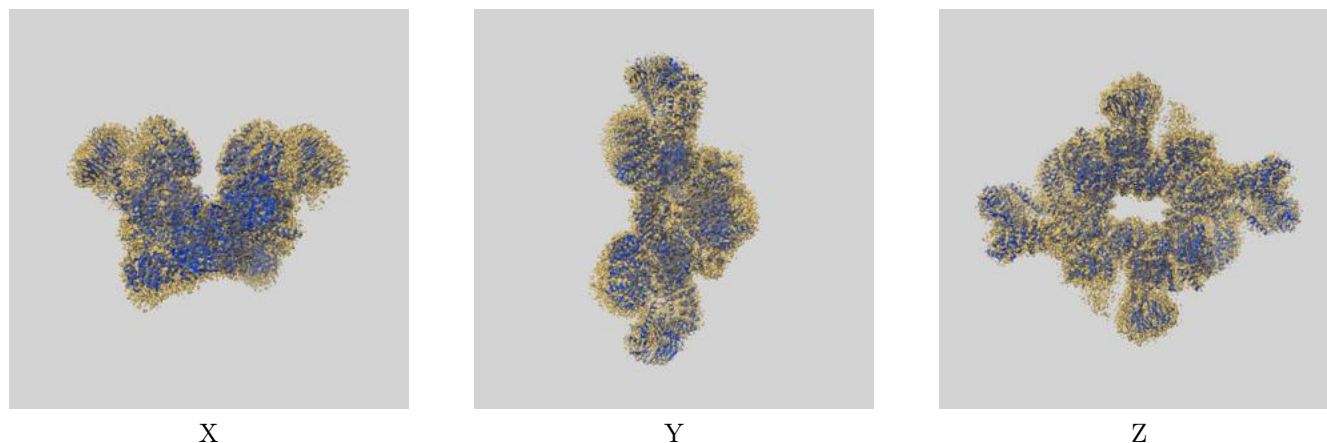
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

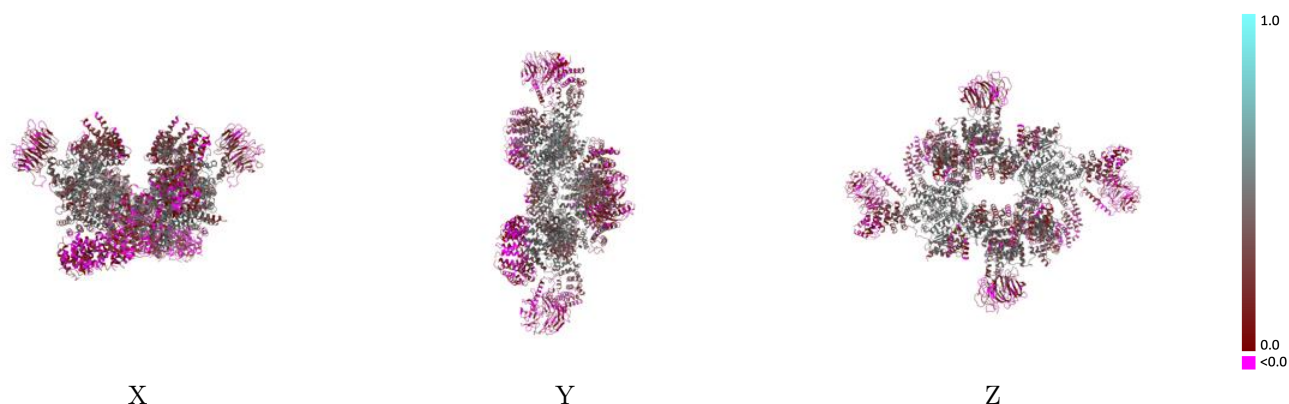
This section contains information regarding the fit between EMDB map EMD-7087 and PDB model 6BCX. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



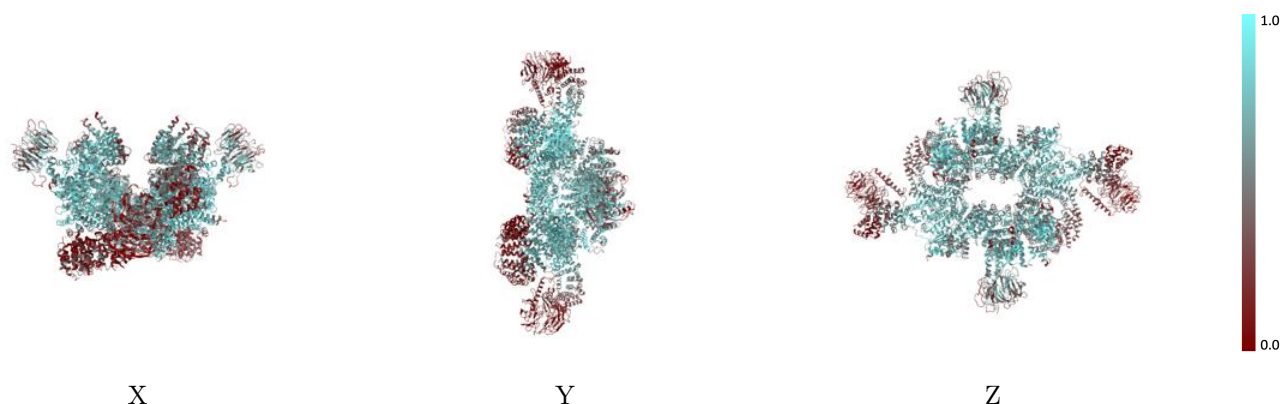
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



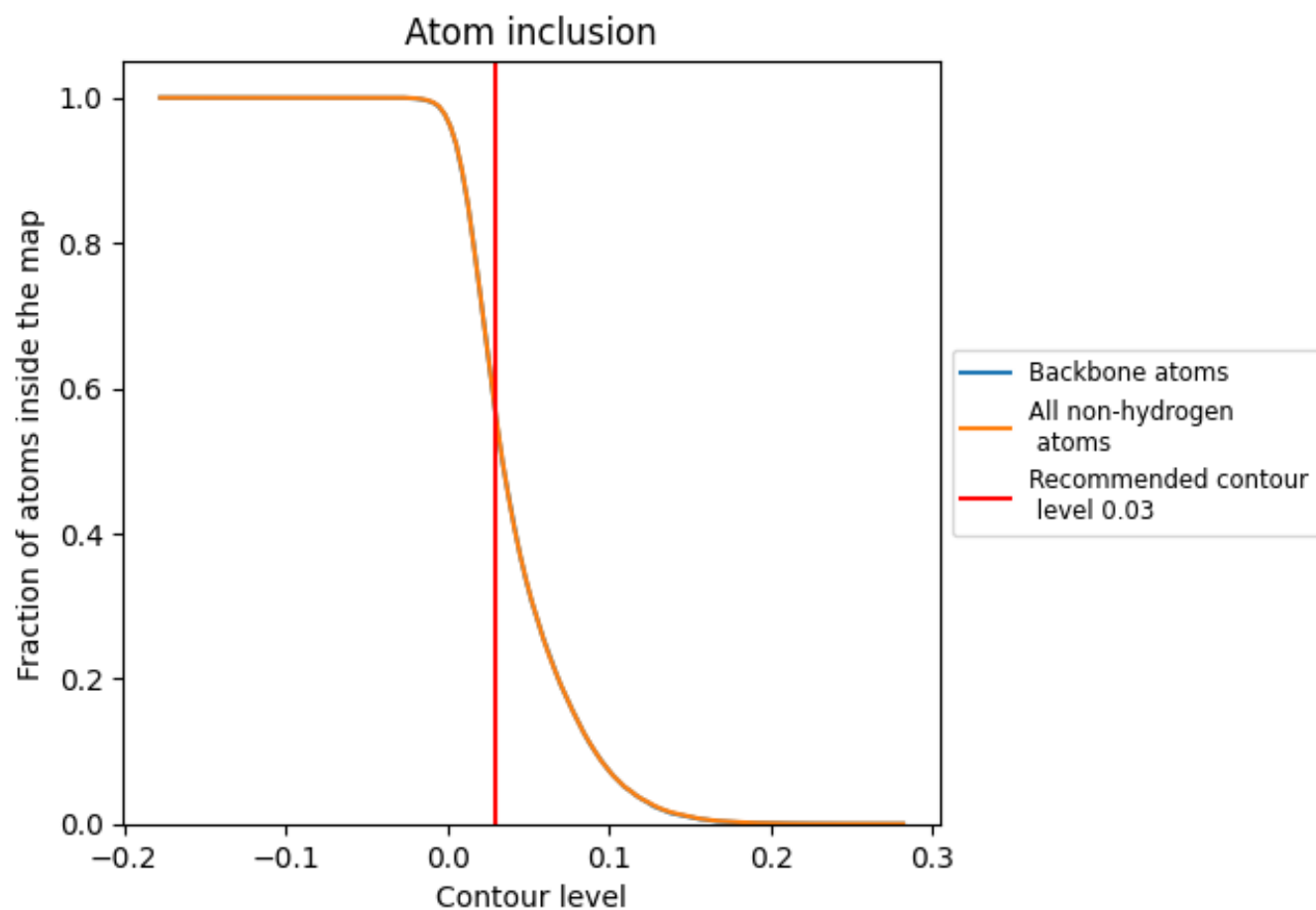
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 56% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5599	<div></div> 0.2750
A	<div></div> 0.6337	<div></div> 0.3120
B	<div></div> 0.6307	<div></div> 0.3100
D	<div></div> 0.4587	<div></div> 0.1190
E	<div></div> 0.4636	<div></div> 0.1270
W	<div></div> 0.4595	<div></div> 0.2440
X	<div></div> 0.6176	<div></div> 0.3600
Y	<div></div> 0.4578	<div></div> 0.2470
Z	<div></div> 0.6029	<div></div> 0.3710

1.0

0.0

<0.0