



## wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 12:56 PM EST

PDB ID : 7UXC  
EMDB ID : EMD-26857  
Title : cryo-EM structure of the mTORC1-TFEB-Rag-Ragulator complex with symmetry expansion  
Authors : Cui, Z.; Hurley, J.  
Deposited on : 2022-05-05  
Resolution : 3.20 Å(reported)

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

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<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

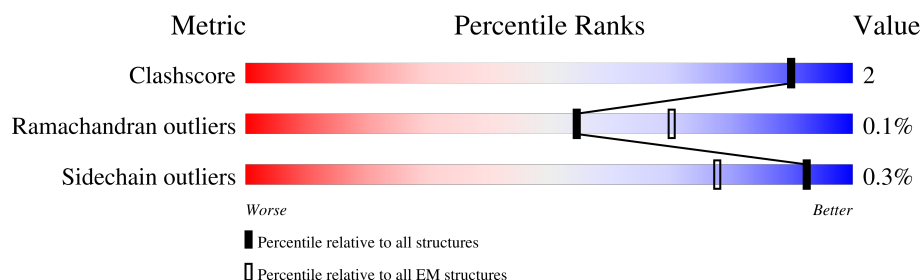
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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>25%</div> <div>83%</div> <div>14%</div> </div>
2	B	326	<div> <div>58%</div> <div>92%</div> <div>5%</div> </div>
3	C	1335	<div> <div>81%</div> <div>15%</div> </div>
4	D	313	<div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
4	K	313	<div> <div>11%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
5	E	399	<div> <div>67%</div> <div>30%</div> </div>
5	L	399	<div> <div>21%</div> <div>64%</div> <div>6%</div> <div>31%</div> </div>
6	F	161	<div> <div>53%</div> <div>65%</div> <div>31%</div> </div>

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Mol	Chain	Length	Quality of chain
6	M	161	
7	G	125	
7	N	125	
8	H	124	
8	O	124	
9	I	99	
9	P	99	
10	J	91	
10	Q	91	
11	R	476	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 95193 atoms, of which 47611 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	2188	Total	C	H	N	O	S	0	0
			35404	11226	17817	3080	3164	117		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	317	Total	C	H	N	O	S	0	0
			4797	1526	2341	436	476	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	1133	Total	C	H	N	O	S	0	0
			18025	5757	9002	1568	1638	60		

- Molecule 4 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	298	Total	C	H	N	O	S	0	0
			4882	1553	2438	427	447	17		
4	K	298	Total	C	H	N	O	S	0	0
			4889	1554	2443	427	448	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	66	LEU	GLN	conflict	UNP Q7L523
K	66	LEU	GLN	conflict	UNP Q7L523

- Molecule 5 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	281	Total	C	H	N	O	S	0	0
			4523	1459	2258	370	424	12		
5	L	277	Total	C	H	N	O	S	0	0
			4446	1430	2220	365	419	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	75	ASN	SER	engineered mutation	UNP Q9HB90
L	75	ASN	SER	engineered mutation	UNP Q9HB90

- Molecule 6 is a protein called Regulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	111	Total	C	H	N	O	S	0	0
			1738	547	870	150	170	1		
6	M	115	Total	C	H	N	O	S	0	0
			1791	562	896	155	176	2		

- Molecule 7 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	124	Total	C	H	N	O	S	0	0
			1888	590	950	161	180	7		
7	N	124	Total	C	H	N	O	S	0	0
			1888	590	950	161	180	7		

- Molecule 8 is a protein called Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	120	Total	C	H	N	O	S	0	0
			1892	601	958	157	175	1		
8	O	120	Total	C	H	N	O	S	0	0
			1892	601	958	157	175	1		

- Molecule 9 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	84	Total	C	H	N	O	S	0	0
			1294	404	652	115	122	1		
9	P	84	Total	C	H	N	O	S	0	0
			1294	404	652	115	122	1		

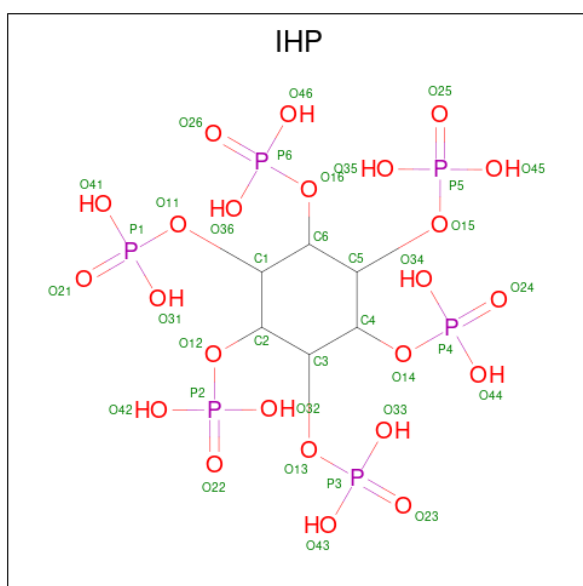
- Molecule 10 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	89	Total	C	H	N	O	S	
			1311	400	656	113	135	7	0
10	Q	89	Total	C	H	N	O	S	
			1311	400	656	113	135	7	0

- Molecule 11 is a protein called Transcription factor EB.

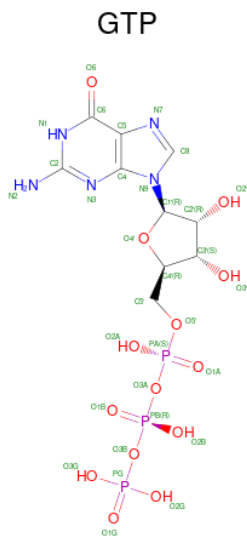
Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	107	Total	C	H	N	O	S	
			1724	541	848	165	165	5	0

- Molecule 12 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	H	O	P	
			42	6	6	24	6	0

- Molecule 13 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

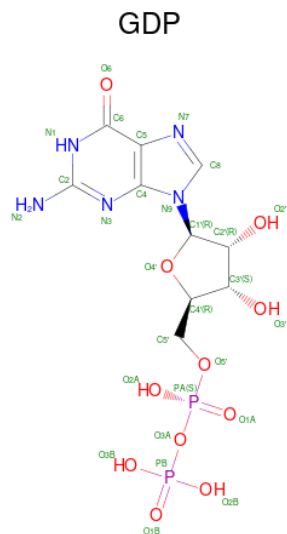


Mol	Chain	Residues	Atoms						AltConf
13	D	1	Total 42	C 10	H 10	N 5	O 14	P 3	0
13	K	1	Total 42	C 10	H 10	N 5	O 14	P 3	0

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
14	D	1	Total Mg 1 1	0
14	K	1	Total Mg 1 1	0

- Molecule 15 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



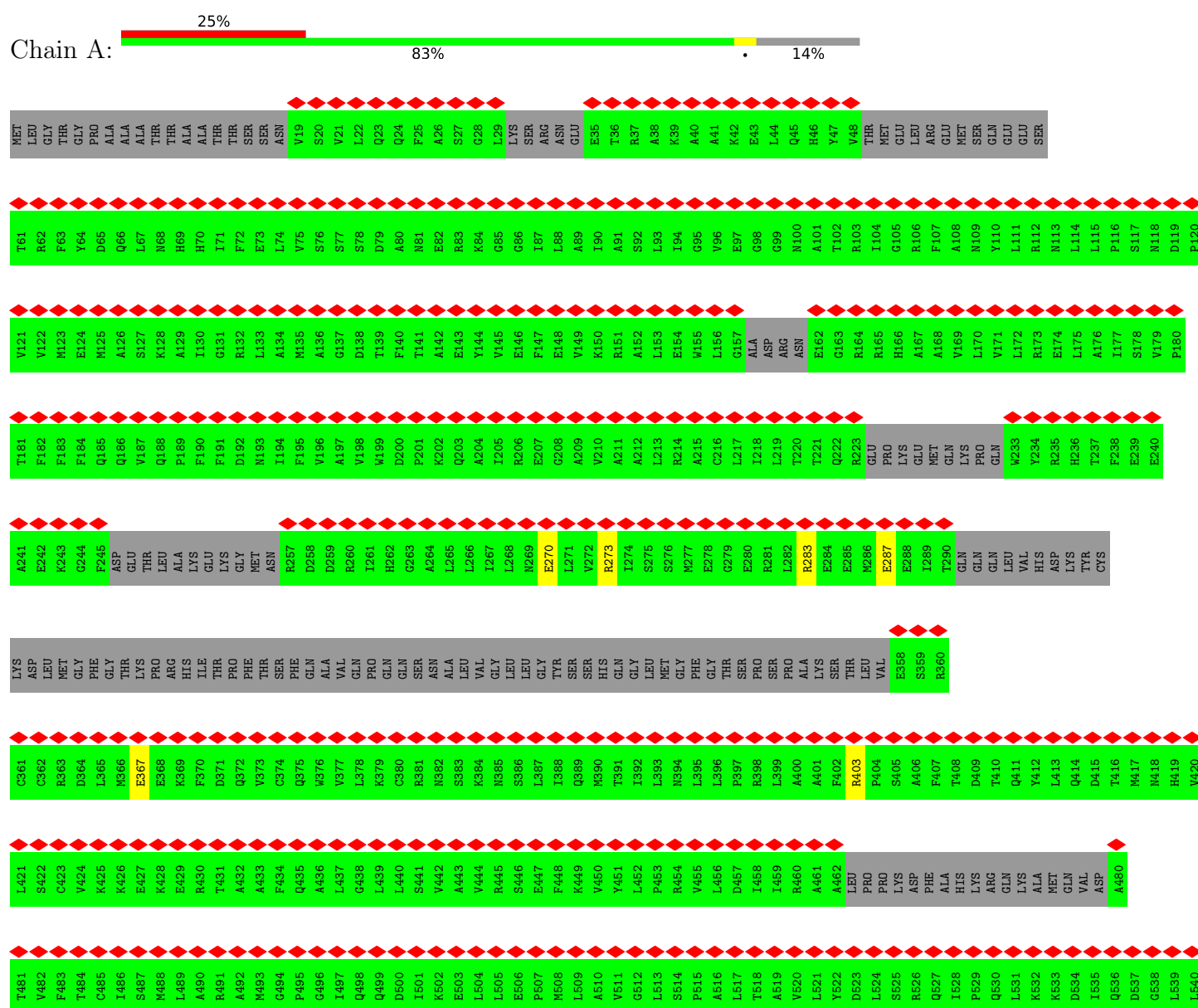
Mol	Chain	Residues	Atoms						AltConf
15	E	1	Total 38	C 10	H 10	N 5	O 11	P 2	0
15	L	1	Total 38	C 10	H 10	N 5	O 11	P 2	0

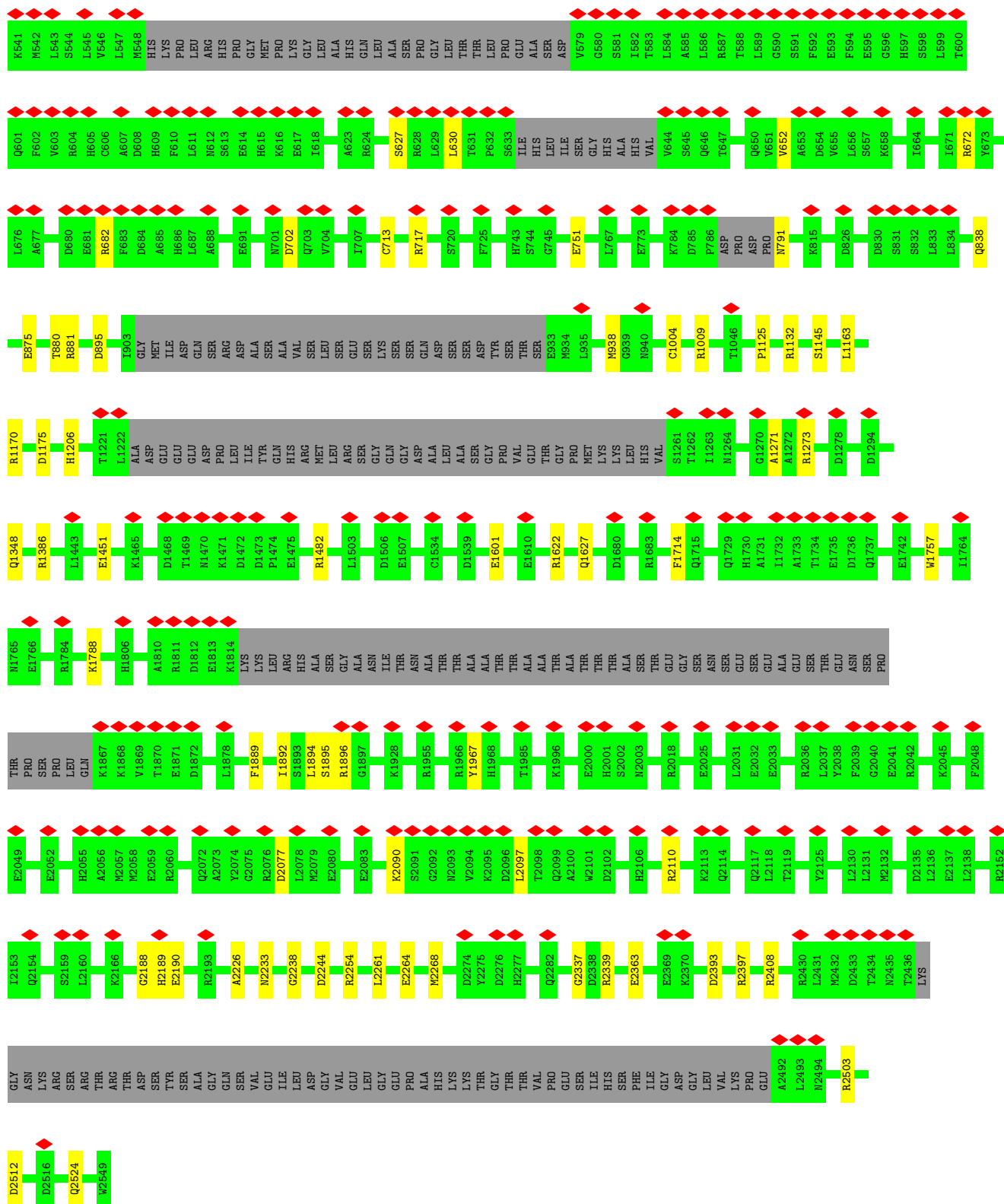


### 3 Residue-property plots

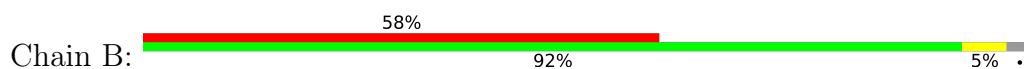
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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





- Molecule 2: Target of rapamycin complex subunit LST8







HIS  
GLN  
THR  
SER  
ALA  
SER  
SER  
LEU  
LYS  
ALA  
LEU  
THR  
HIS  
ASN  
GLY  
THR  
PRO  
ARG  
ASN  
ALA  
ILE

• Molecule 6: Regulator complex protein LAMTOR1

Chain F: 53% 65% 31%

MET  
GLY  
CYS  
TYR  
SER  
SER  
GLU  
ASN  
GLU  
ASP  
SER  
ASP  
GLN  
ASP  
ARG  
GLU  
GLU  
LYS  
LEU  
LEU  
LEU  
ASP  
PRO  
SER  
SER  
PRO  
PRO  
THR  
LYS  
ALA  
LEU  
ASN  
GLY  
ALA  
GLU  
PRO  
ASN  
TYR  
HIS  
SER  
LEU  
PRO  
SER  
ALA  
R47  
T48  
D49  
E50  
Q51  
A52  
S69  
A70  
A71  
D72  
SER  
GLN  
GLY

MET  
E77  
Q78  
H79  
E80  
Y81  
M82  
D83  
R84  
A85  
R86  
Q87  
Y88  
S89  
T90  
R91  
L92  
A93  
V94  
L95  
V155  
S96  
S97  
S98  
L99  
T100  
H101  
W102  
K103  
K104  
L105  
P106  
P107  
L108  
P109  
S110  
L111  
T112  
S113  
Q114  
P115  
H116  
Q117  
V118  
L119  
A120  
S121  
E122  
P123  
I124  
P125  
F126  
D128  
L129  
Q130  
Q131  
V132  
S133  
R134  
I135

A136  
A137  
Y138  
A139  
Y140  
S141  
A142  
L143  
S144  
Q145  
I146  
R147  
V148  
D149  
A150  
K151  
E152  
E153  
L154  
V156  
G159  
I160  
P161

• Molecule 6: Regulator complex protein LAMTOR1

Chain M: 48% 63% 9% 29%

MET  
GLY  
CYS  
TYR  
SER  
SER  
GLU  
ASN  
GLU  
ASP  
SER  
ASP  
GLN  
ASP  
ARG  
GLU  
ARG  
LYS  
LEU  
LEU  
LEU  
ASP  
PRO  
SER  
SER  
SER  
PRO  
PRO  
THR  
LYS  
ALA  
LEU  
ASN  
GLY  
ALA  
GLU  
PRO  
ASN  
TYR  
HIS  
SER  
LEU  
PRO  
SER  
ALA  
R47  
T48  
D49  
E50  
Q51  
A52  
D67  
V68  
S69  
A70  
A71  
D72  
S73

Q74  
G75  
M76  
E77  
E80  
D83  
R84  
A85  
R86  
Q87  
Y88  
R91  
L92  
L95  
S96  
S97  
S98  
L99  
T100  
H101  
W102  
L105  
P106  
P107  
L108  
P109  
S110  
L111  
T112  
S113  
Q114  
P115  
H116  
Q117  
V118  
L119  
A120  
S121  
E122  
P123  
I124  
P125  
F126  
D128  
L129  
Q130  
Q131  
V132  
S133  
R134  
I135  
A137  
Y138

A139  
Y140  
S141  
A142  
L143  
S144  
Q145  
I146  
R147  
D149  
A150  
K151  
E152  
E153  
L154  
V155  
V156  
Q157  
F158  
G159  
I160  
P161

• Molecule 7: Regulator complex protein LAMTOR2

Chain G: 35% 92% 7%

M1  
L2  
R3  
P4  
K5  
T8  
Q13  
A14  
N15  
T16  
G17  
G18  
V19  
Q20  
S21  
T22  
L23  
Y37  
G38  
D39  
T40  
D41  
A46  
A54  
D57  
R58  
N59  
G60  
N61  
Q62  
A63  
F64  
N65  
E66  
D67  
N68  
L69  
K70  
M74  
M77  
E78  
A82  
I83  
T84  
R85  
V86  
M93  
K96  
E97

T98  
V99  
G100  
F101  
G102  
M103  
L104  
K105  
A106  
Q109  
Q113  
E117  
Q121  
A124  
SER

• Molecule 7: Regulator complex protein LAMTOR2

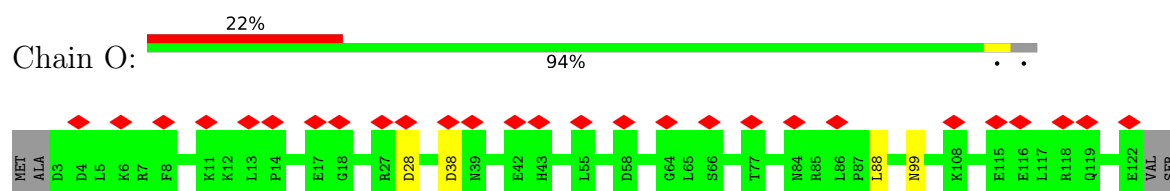
Chain N: 23% 93% 6%

M1  
L2  
R3  
P4  
K5  
T8  
Q9  
V10  
L11  
S12  
Q13  
A14  
N15  
T16  
G17  
G18  
E28  
Y37  
G38  
D39  
T40  
D41  
R58  
N61  
Q62  
F64  
N65  
E66  
D67  
E78  
Q79  
V86  
K96  
E97  
T98  
V99  
G100  
Q113  
E117  
T120  
Q121  
V122  
A123  
A124  
SER

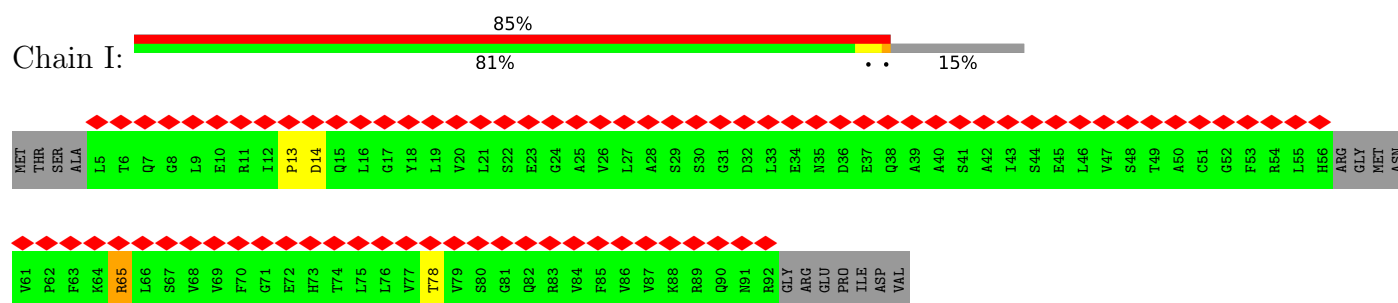
- Molecule 8: Regulator complex protein LAMTOR3



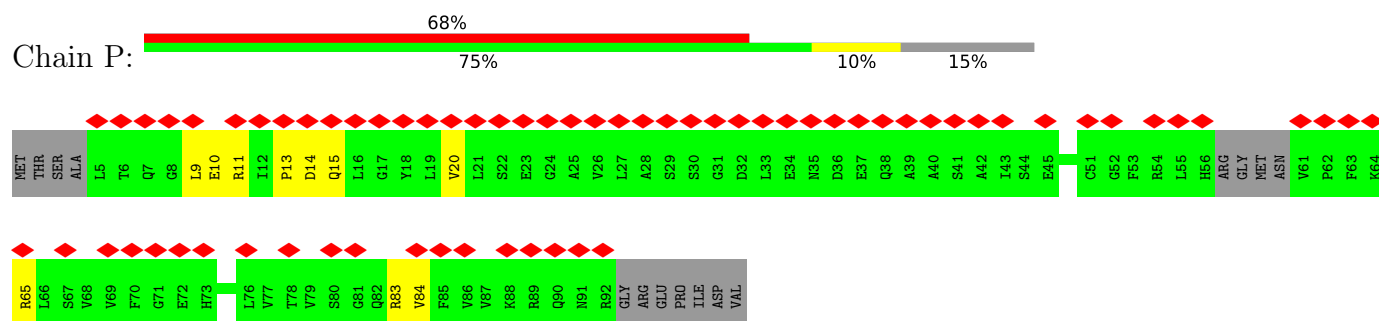
- Molecule 8: Regulator complex protein LAMTOR3



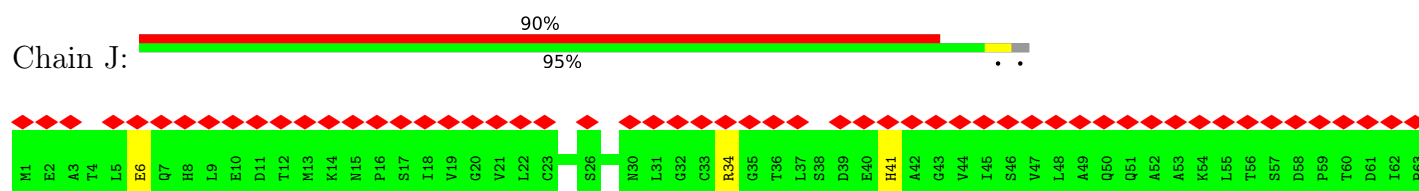
- Molecule 9: Regulator complex protein LAMTOR4

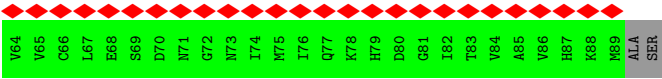


- Molecule 9: Regulator complex protein LAMTOR4

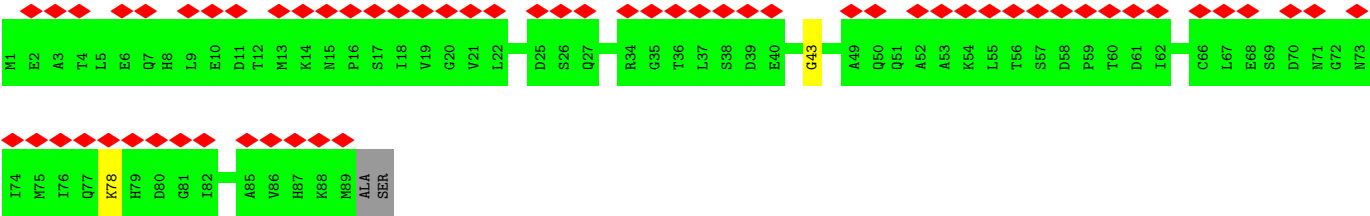


- Molecule 10: Regulator complex protein LAMTOR5

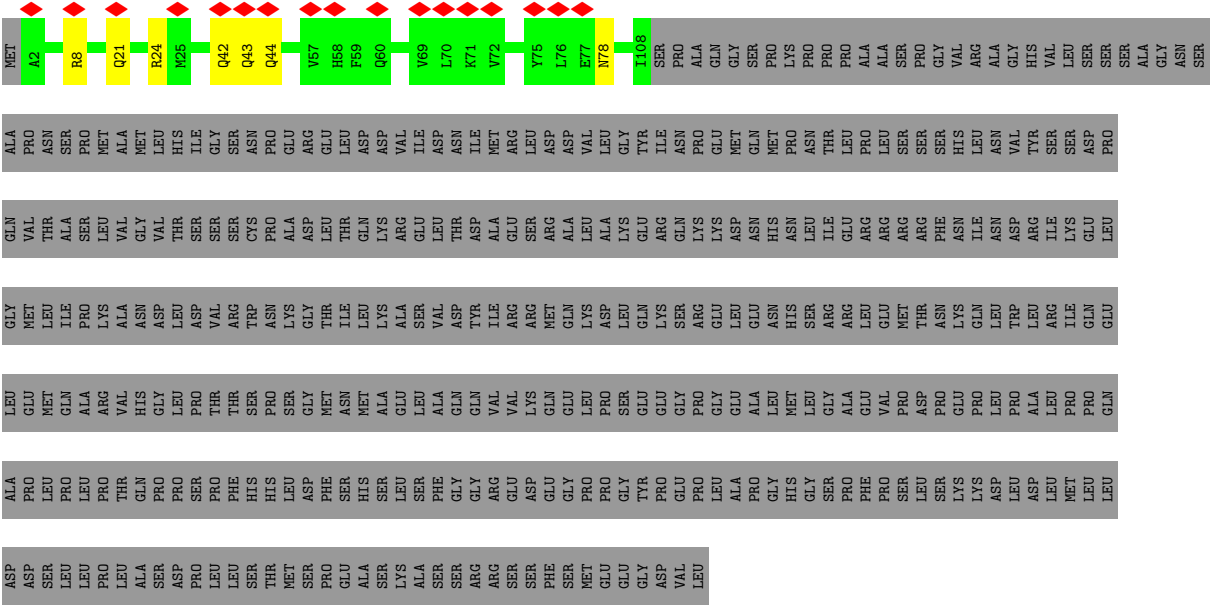




• Molecule 10: Regulator complex protein LAMTOR5



• Molecule 11: Transcription factor EB



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192332	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.985	Depositor
Minimum map value	-1.752	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	617.39996, 617.39996, 617.39996	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GDP, MG, IHP

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	0.28	0/17941	0.60	2/24276 (0.0%)
2	B	0.26	0/2514	0.57	0/3426
3	C	0.29	0/9242	0.61	1/12573 (0.0%)
4	D	0.29	0/2489	0.64	0/3350
4	K	0.30	0/2491	0.67	1/3353 (0.0%)
5	E	0.31	0/2309	0.62	0/3114
5	L	0.30	0/2267	0.61	0/3057
6	F	0.28	0/884	0.64	0/1201
6	M	0.29	0/912	0.63	0/1239
7	G	0.30	0/949	0.70	0/1285
7	N	0.32	0/949	0.70	0/1285
8	H	0.29	0/951	0.65	0/1290
8	O	0.30	0/951	0.69	2/1290 (0.2%)
9	I	0.27	0/649	0.63	0/876
9	P	0.27	0/649	0.67	0/876
10	J	0.27	0/661	0.57	0/896
10	Q	0.28	0/661	0.64	0/896
11	R	0.30	0/896	0.65	0/1211
All	All	0.29	0/48365	0.62	6/65494 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
4	D	0	1
9	I	0	1
9	P	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	O	88	LEU	CA-CB-CG	5.49	127.92	115.30
8	O	88	LEU	CB-CG-CD2	5.34	120.08	111.00
1	A	1967	TYR	CA-CB-CG	5.18	123.25	113.40
3	C	796	LEU	CA-CB-CG	5.07	126.97	115.30
1	A	2097	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	118	ARG	Sidechain
3	C	188	SER	Peptide
4	D	227	ARG	Sidechain
9	I	65	ARG	Sidechain
9	P	65	ARG	Sidechain

## 5.2 Too-close contacts

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	17587	17817	17819	38	0
2	B	2456	2341	2341	9	0
3	C	9023	9002	9000	28	0
4	D	2444	2438	2438	8	0
4	K	2446	2443	2443	13	0
5	E	2265	2258	2258	9	0
5	L	2226	2220	2220	15	0
6	F	868	870	870	4	0
6	M	895	896	896	11	0
7	G	938	950	950	7	0
7	N	938	950	950	4	0
8	H	934	958	958	9	0
8	O	934	958	958	3	0
9	I	642	652	652	2	0
9	P	642	652	652	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	655	656	656	2	0
10	Q	655	656	656	1	0
11	R	876	848	847	4	0
12	A	36	6	6	1	0
13	D	32	10	12	0	0
13	K	32	10	12	0	0
14	D	1	0	0	0	0
14	K	1	0	0	0	0
15	E	28	10	12	0	0
15	L	28	10	12	3	0
All	All	47582	47611	47618	160	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 2.

The worst 5 of 160 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)
5:E:327:TYR:OH	5:E:353:ASP:OD1	1.97	0.82
3:C:1207:TYR:OH	3:C:1243:MET:O	2.00	0.79
5:L:198:ARG:NH1	5:L:202:ASP:OD2	2.17	0.77
3:C:790:ALA:O	3:C:794:SER:OG	2.02	0.77
10:J:6:GLU:OE1	10:J:34:ARG:NH2	2.20	0.75

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	2158/2549 (85%)	2108 (98%)	50 (2%)	0	100	100
2	B	315/326 (97%)	297 (94%)	18 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	1123/1335 (84%)	1050 (94%)	73 (6%)	0	100	100
4	D	296/313 (95%)	283 (96%)	13 (4%)	0	100	100
4	K	296/313 (95%)	273 (92%)	22 (7%)	1 (0%)	41	74
5	E	275/399 (69%)	261 (95%)	14 (5%)	0	100	100
5	L	271/399 (68%)	258 (95%)	13 (5%)	0	100	100
6	F	107/161 (66%)	101 (94%)	6 (6%)	0	100	100
6	M	113/161 (70%)	105 (93%)	8 (7%)	0	100	100
7	G	122/125 (98%)	118 (97%)	3 (2%)	1 (1%)	19	58
7	N	122/125 (98%)	115 (94%)	6 (5%)	1 (1%)	19	58
8	H	118/124 (95%)	111 (94%)	7 (6%)	0	100	100
8	O	118/124 (95%)	116 (98%)	2 (2%)	0	100	100
9	I	80/99 (81%)	69 (86%)	10 (12%)	1 (1%)	12	47
9	P	80/99 (81%)	69 (86%)	10 (12%)	1 (1%)	12	47
10	J	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
10	Q	87/91 (96%)	80 (92%)	7 (8%)	0	100	100
11	R	105/476 (22%)	99 (94%)	5 (5%)	1 (1%)	15	54
All	All	5873/7310 (80%)	5592 (95%)	275 (5%)	6 (0%)	54	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	86	VAL
7	N	86	VAL
11	R	43	GLN
9	P	13	PRO
4	K	45	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	1919/2220 (86%)	1918 (100%)	1 (0%)	93	98
2	B	269/276 (98%)	269 (100%)	0	100	100
3	C	1000/1163 (86%)	997 (100%)	3 (0%)	92	96
4	D	271/287 (94%)	268 (99%)	3 (1%)	73	88
4	K	272/287 (95%)	270 (99%)	2 (1%)	84	94
5	E	255/340 (75%)	255 (100%)	0	100	100
5	L	251/340 (74%)	250 (100%)	1 (0%)	91	95
6	F	97/141 (69%)	95 (98%)	2 (2%)	53	79
6	M	100/141 (71%)	99 (99%)	1 (1%)	76	90
7	G	97/98 (99%)	97 (100%)	0	100	100
7	N	97/98 (99%)	97 (100%)	0	100	100
8	H	105/108 (97%)	104 (99%)	1 (1%)	76	90
8	O	105/108 (97%)	105 (100%)	0	100	100
9	I	71/83 (86%)	71 (100%)	0	100	100
9	P	71/83 (86%)	71 (100%)	0	100	100
10	J	76/77 (99%)	76 (100%)	0	100	100
10	Q	76/77 (99%)	75 (99%)	1 (1%)	69	87
11	R	96/419 (23%)	96 (100%)	0	100	100
All	All	5228/6346 (82%)	5213 (100%)	15 (0%)	92	96

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	47	ARG
6	M	47	ARG
6	F	151	LYS
10	Q	78	LYS
4	K	295	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2106	HIS

### 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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z  > 2$
12	IHP	A	2601	-	36,36,36	1.47	6 (16%)	54,60,60	0.64	1 (1%)
13	GTP	D	401	14	26,34,34	1.18	2 (7%)	32,54,54	1.62	6 (18%)
13	GTP	K	401	14	26,34,34	1.16	2 (7%)	32,54,54	1.58	6 (18%)
15	GDP	E	401	-	24,30,30	0.92	1 (4%)	30,47,47	1.20	3 (10%)
15	GDP	L	401	-	24,30,30	0.93	1 (4%)	30,47,47	1.21	3 (10%)

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
12	IHP	A	2601	-	-	9/30/54/54	0/1/1/1
13	GTP	D	401	14	-	1/18/38/38	0/3/3/3
13	GTP	K	401	14	-	5/18/38/38	0/3/3/3
15	GDP	E	401	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GDP	L	401	-	-	3/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	K	401	GTP	C5-C6	-4.12	1.39	1.47
13	D	401	GTP	C5-C6	-4.10	1.39	1.47
12	A	2601	IHP	P3-O13	3.59	1.66	1.59
12	A	2601	IHP	P4-O14	3.14	1.65	1.59
12	A	2601	IHP	P2-O12	3.07	1.65	1.59

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	401	GTP	PB-O3B-PG	-4.25	118.23	132.83
13	K	401	GTP	PB-O3B-PG	-3.90	119.44	132.83
13	K	401	GTP	PA-O3A-PB	-3.73	120.03	132.83
13	D	401	GTP	PA-O3A-PB	-3.61	120.42	132.83
15	E	401	GDP	PA-O3A-PB	-3.52	120.75	132.83

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	2601	IHP	C2-C3-O13-P3
12	A	2601	IHP	C3-C4-O14-P4
12	A	2601	IHP	C5-C4-O14-P4
12	A	2601	IHP	C1-C6-O16-P6
12	A	2601	IHP	C5-C6-O16-P6

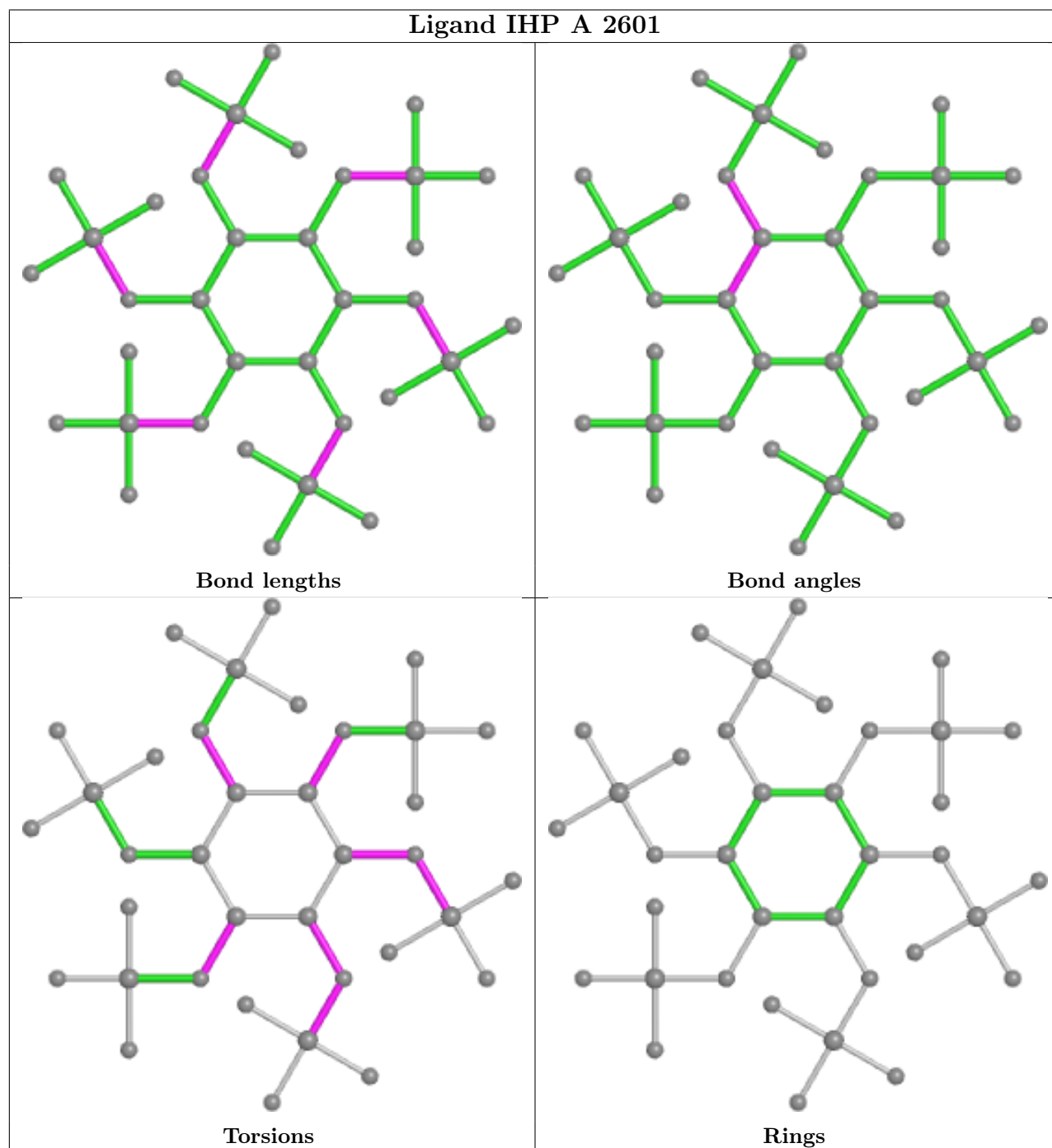
There are no ring outliers.

2 monomers are involved in 4 short contacts:

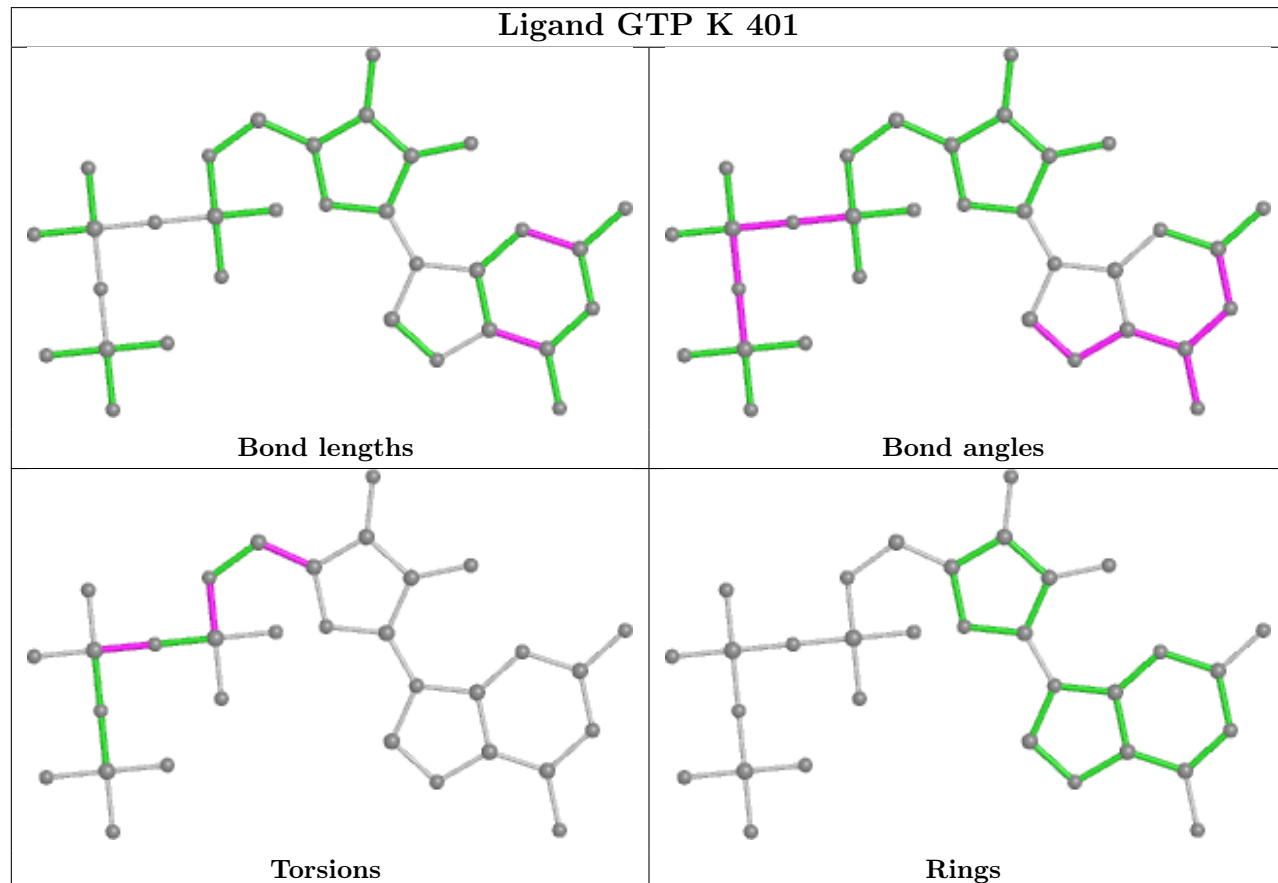
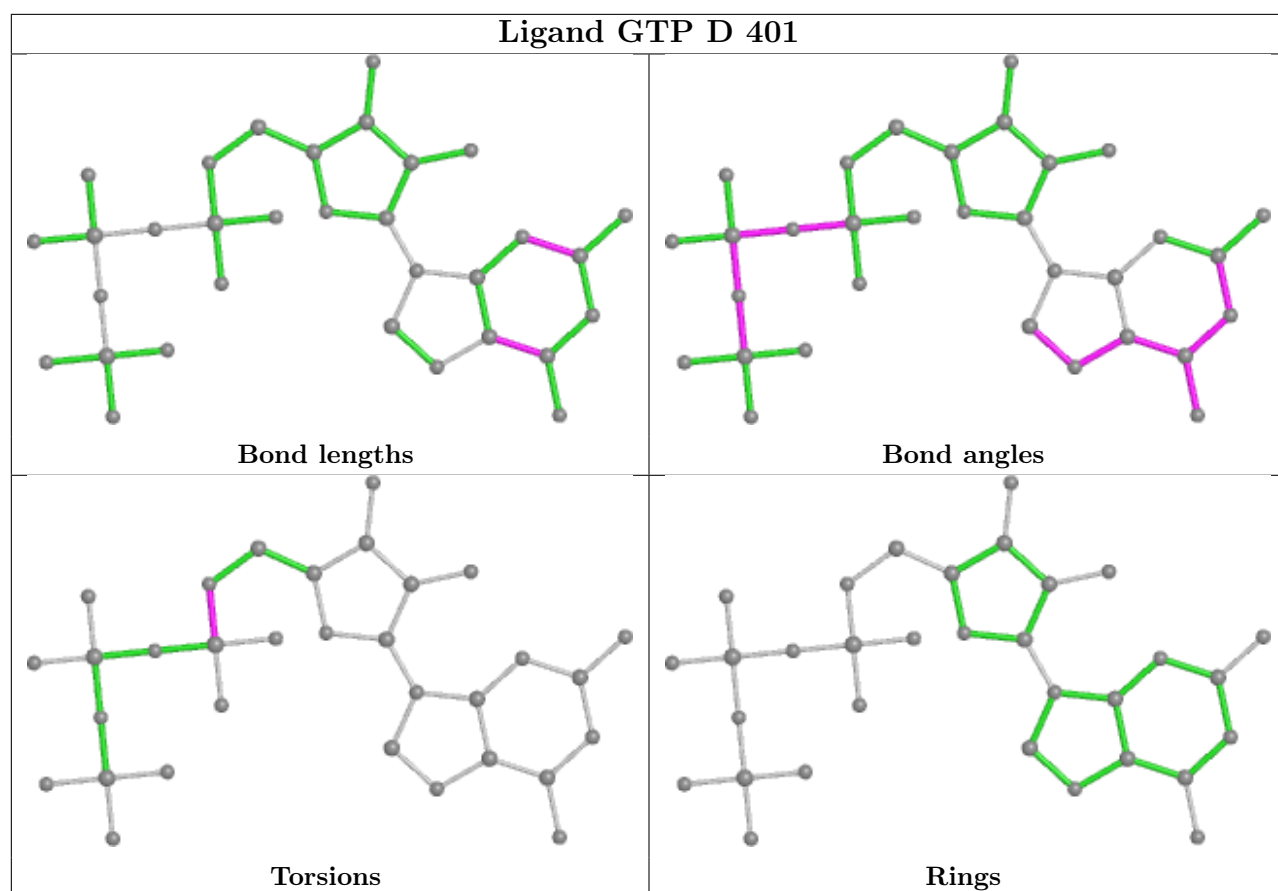
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	2601	IHP	1	0
15	L	401	GDP	3	0

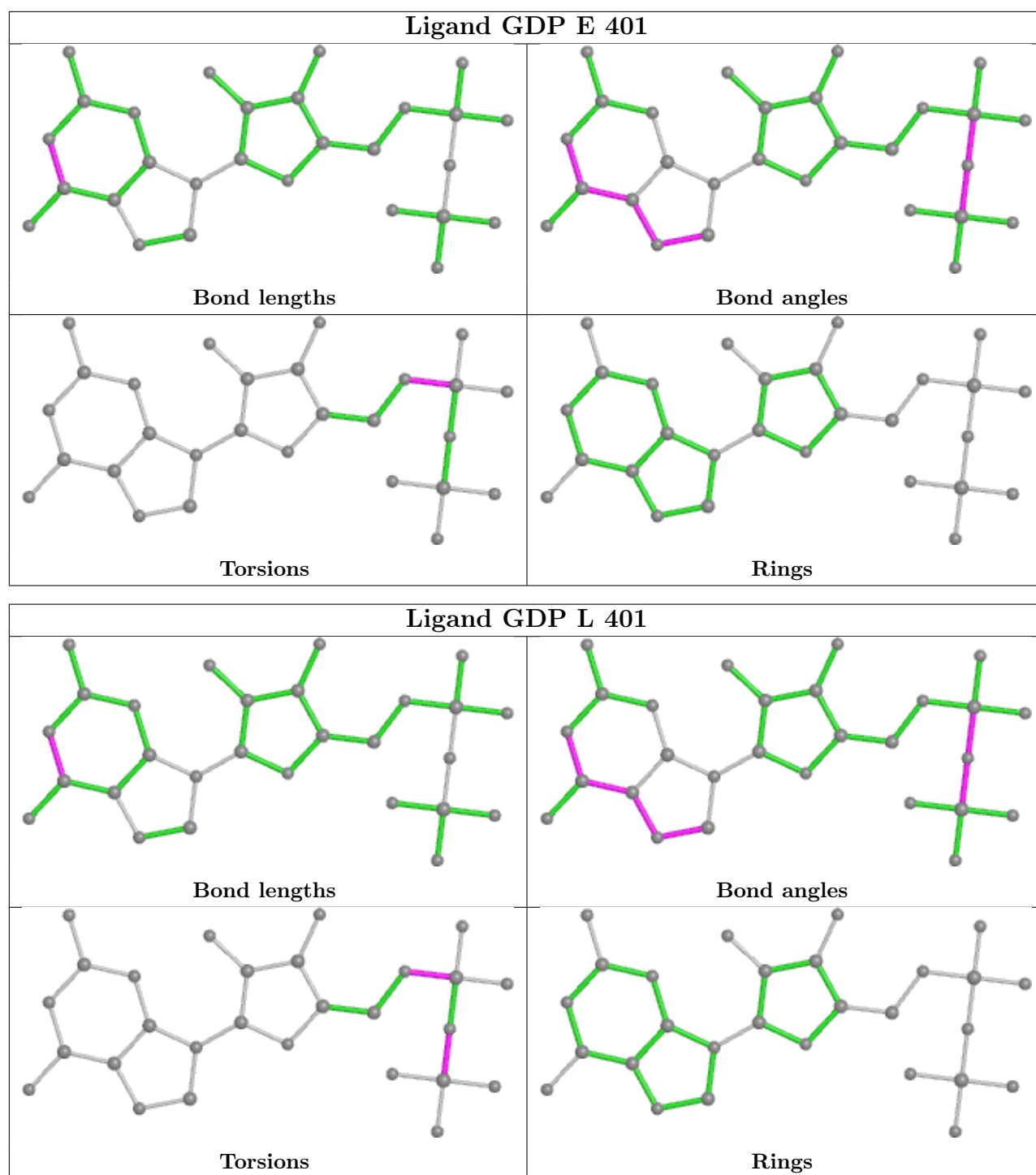
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

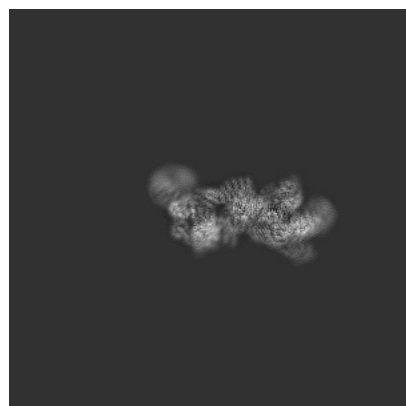
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26857. These allow visual inspection of the internal detail of the map and identification of artifacts.

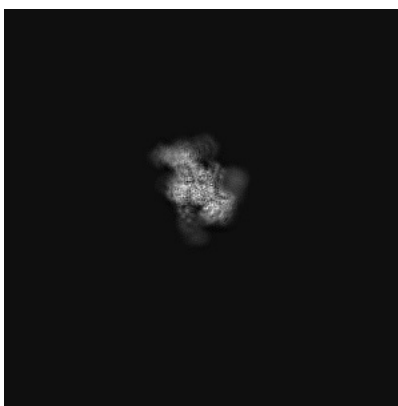
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

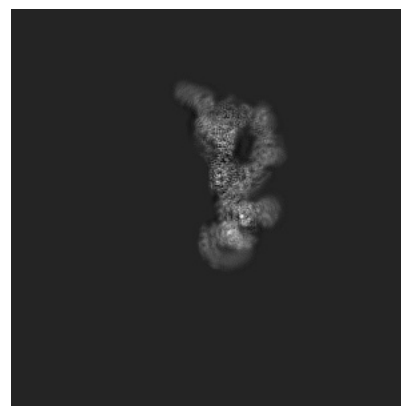
#### 6.1.1 Primary map



X

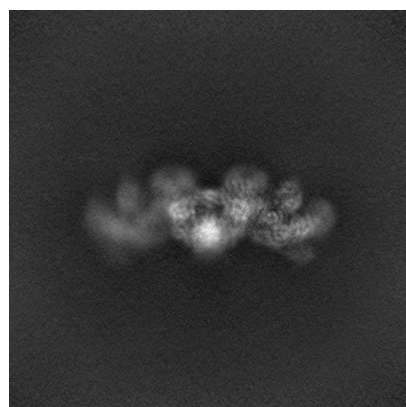


Y

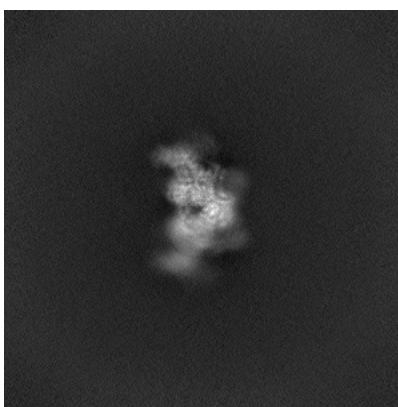


Z

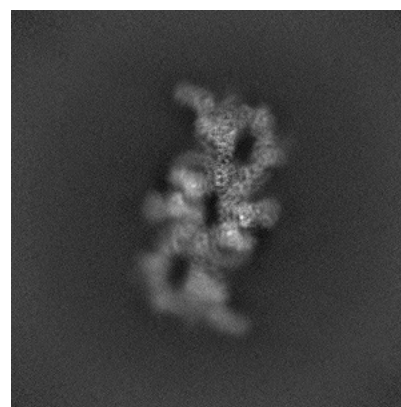
#### 6.1.2 Raw map



X



Y



Z

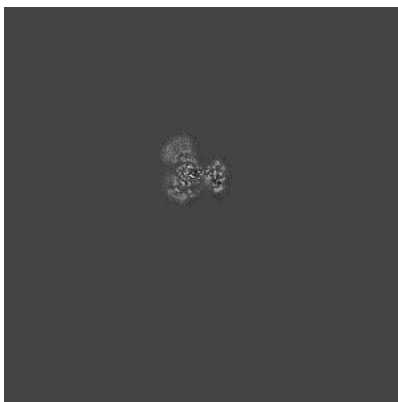
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 294



Y Index: 294



Z Index: 294

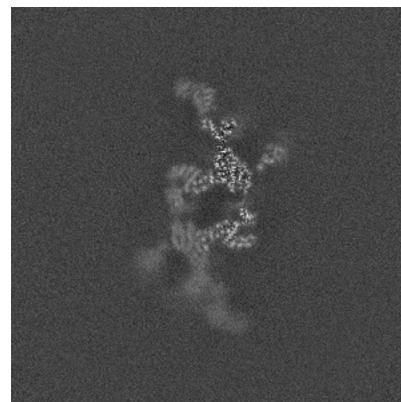
### 6.2.2 Raw map



X Index: 294



Y Index: 294

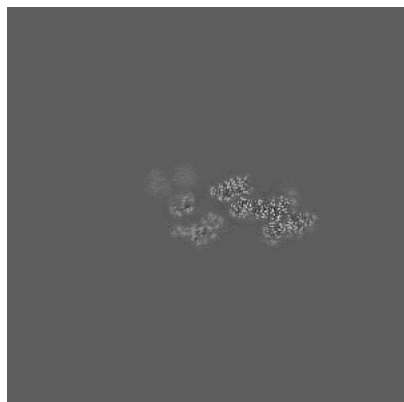


Z Index: 294

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

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

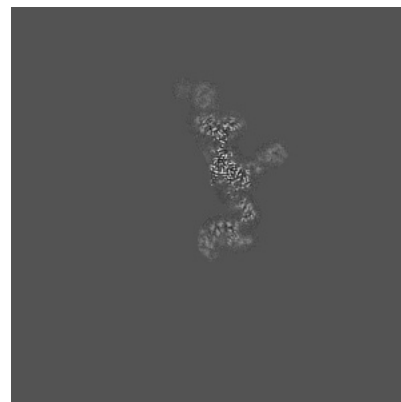
### 6.3.1 Primary map



X Index: 313

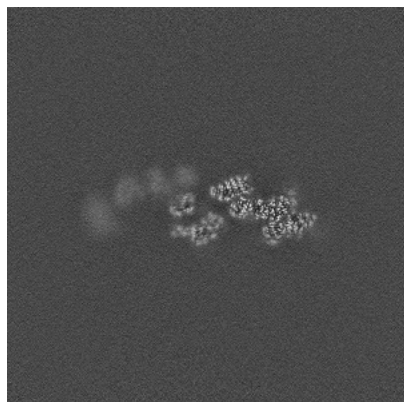


Y Index: 400



Z Index: 300

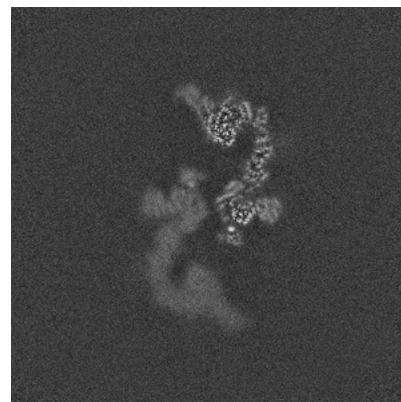
### 6.3.2 Raw map



X Index: 313



Y Index: 292

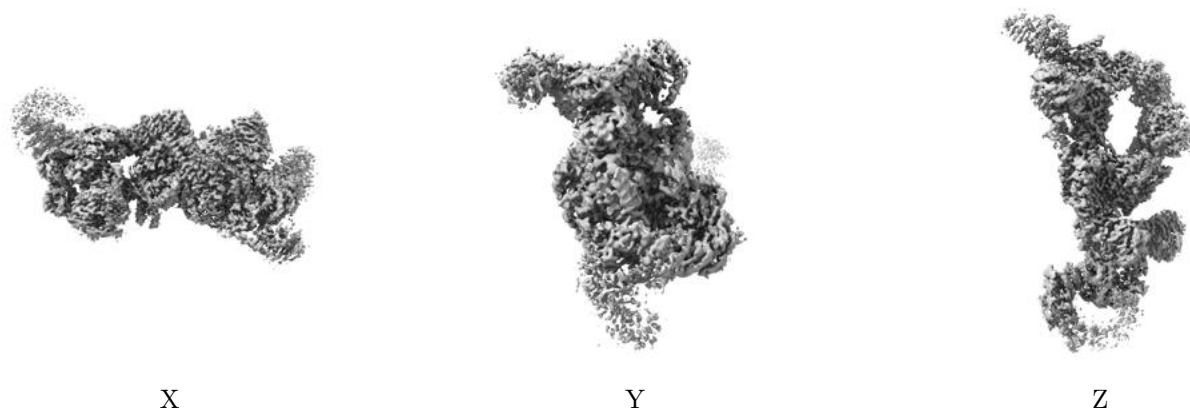


Z Index: 267

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

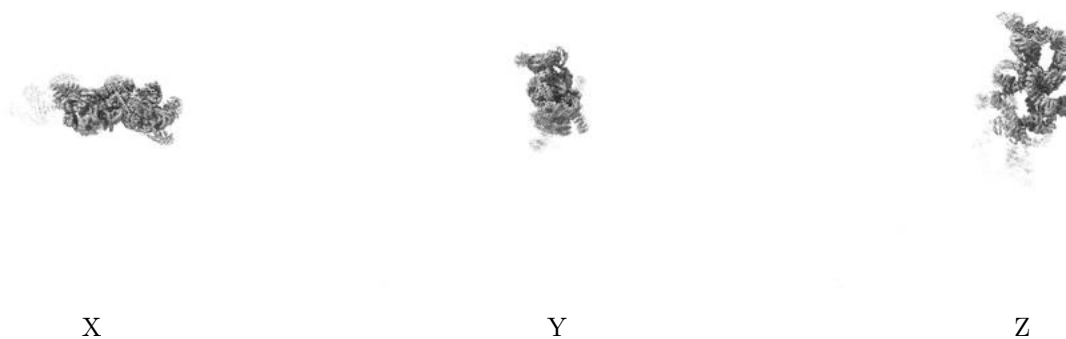
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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.

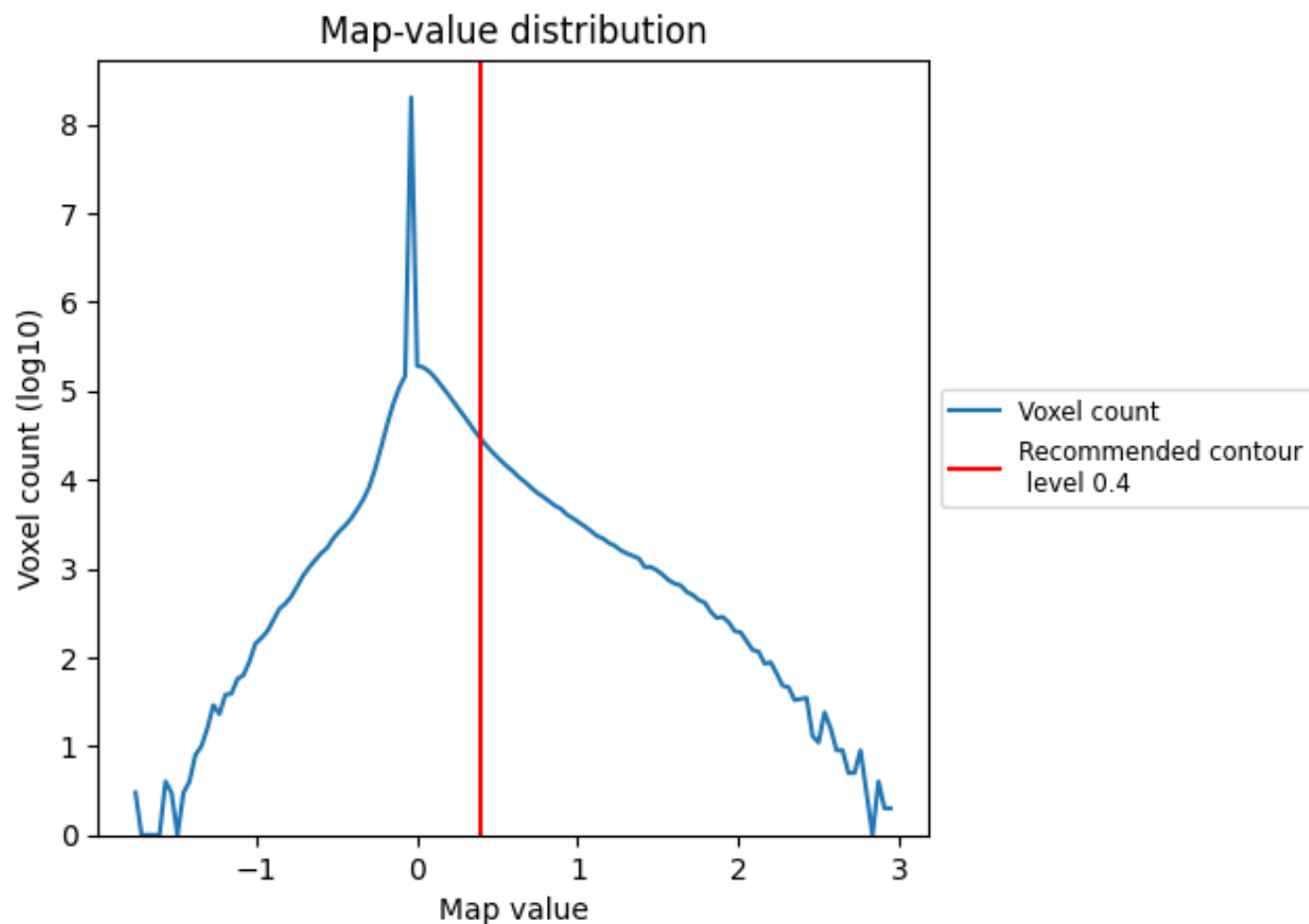
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

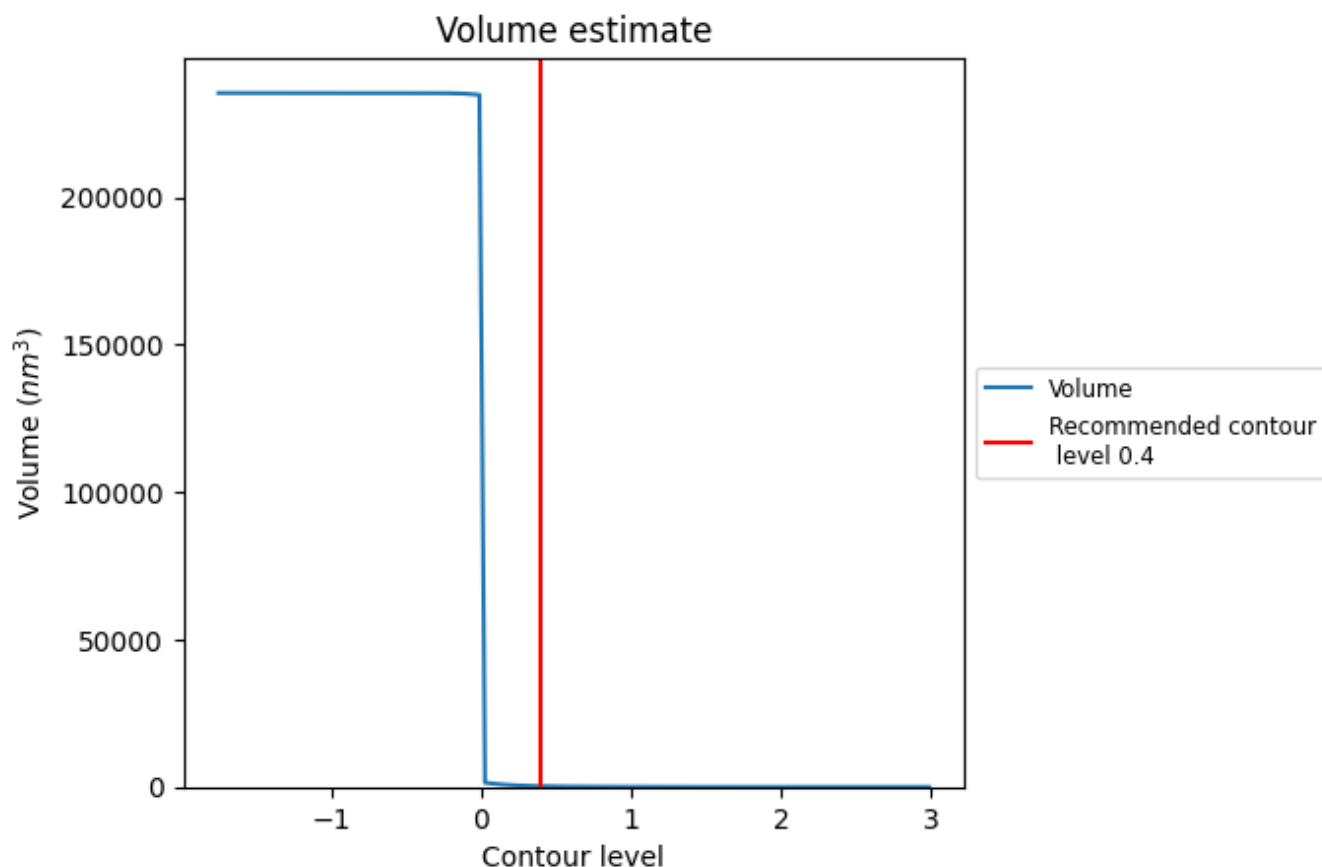
This section contains the results of statistical analysis of the map.

### 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](#)

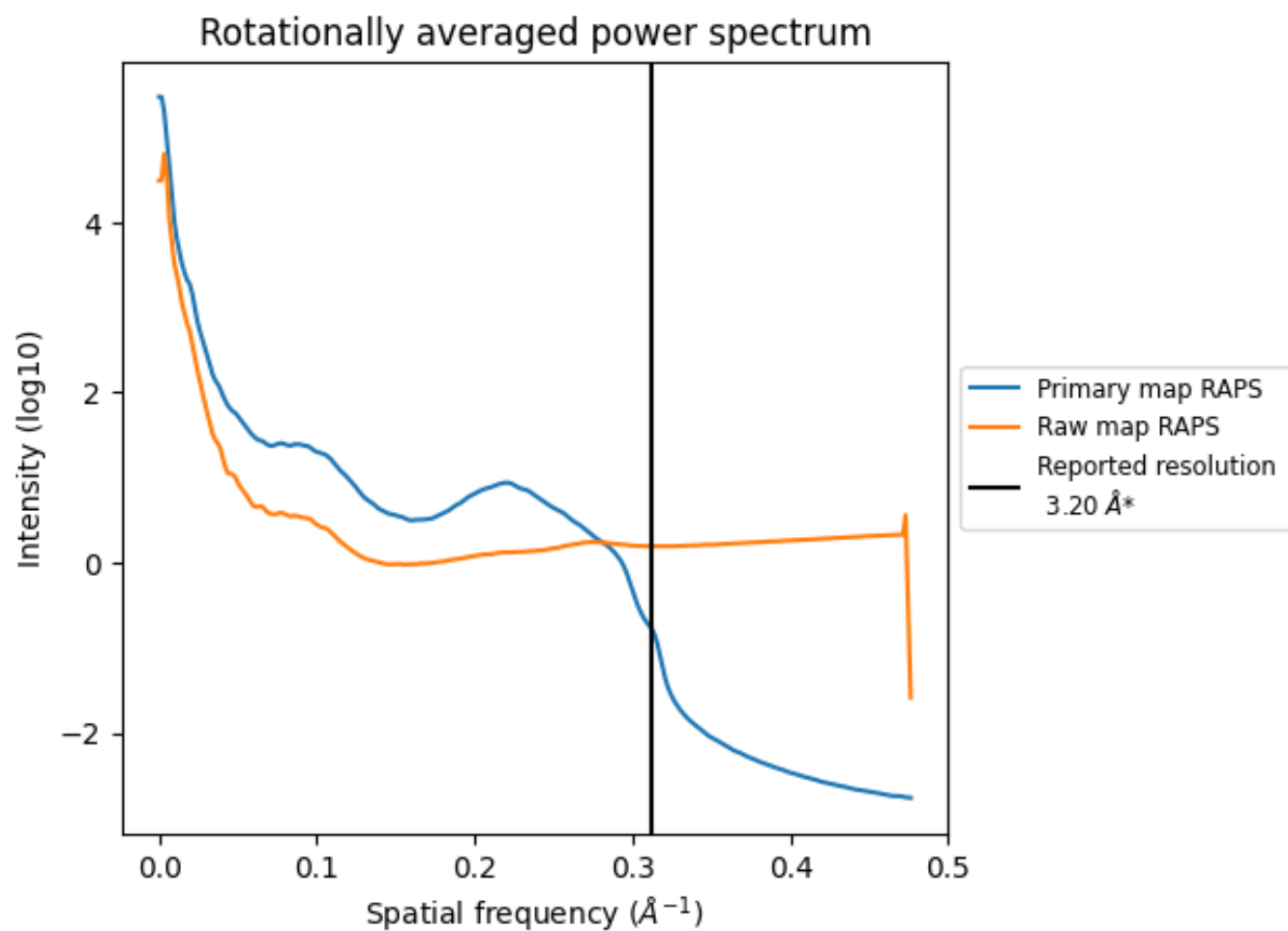


The volume at the recommended contour level is 253 nm<sup>3</sup>; this corresponds to an approximate mass of 229 kDa.

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 ⓘ

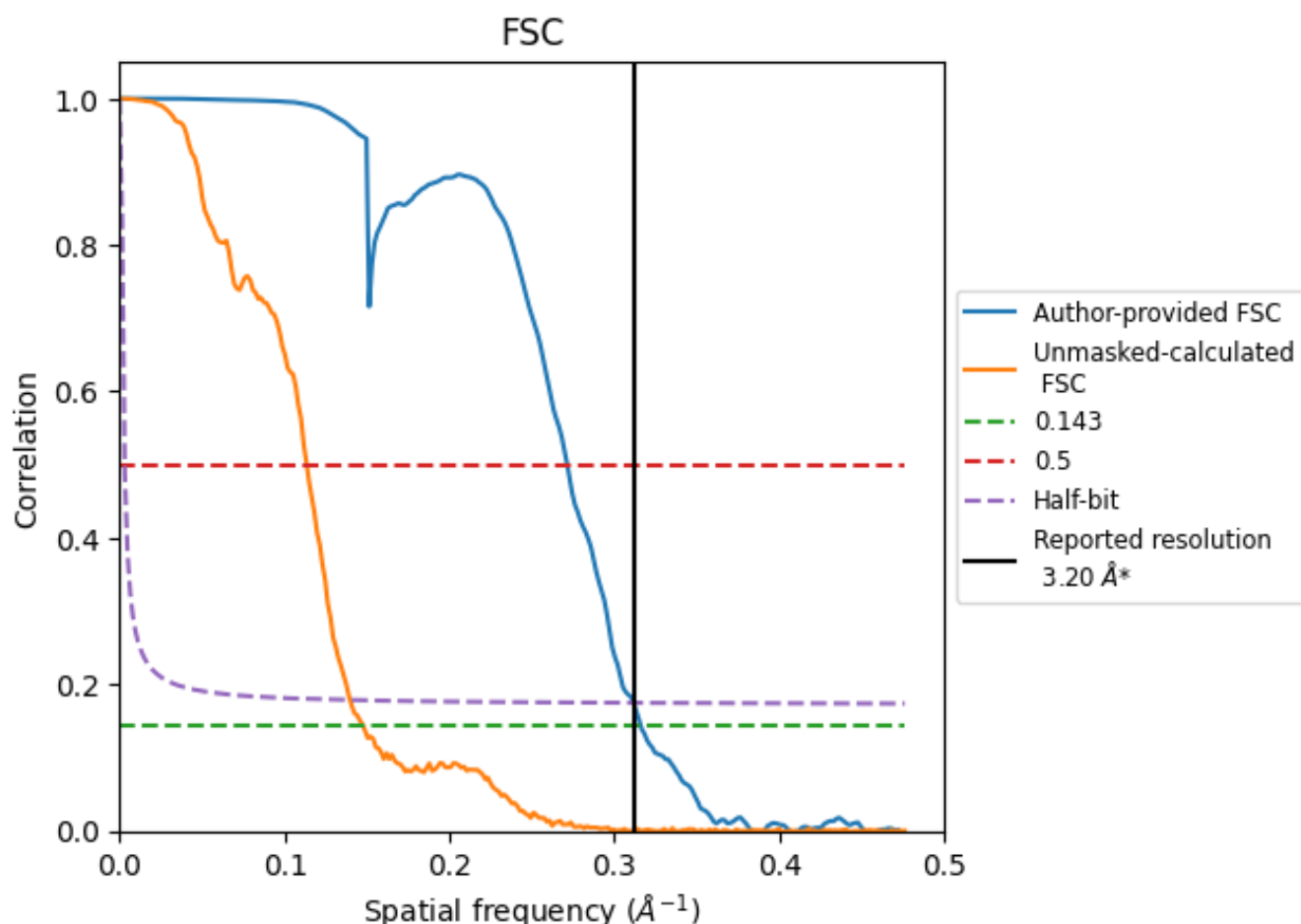


\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

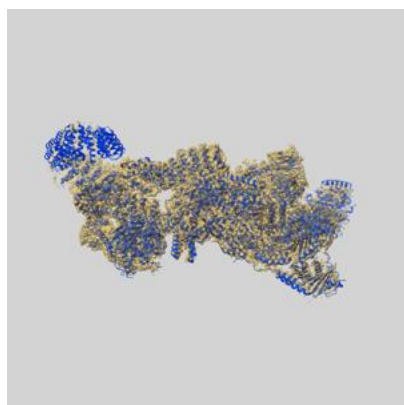
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.16	3.68	3.21
Unmasked-calculated*	6.77	8.81	7.15

\*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 6.77 differs from the reported value 3.2 by more than 10 %

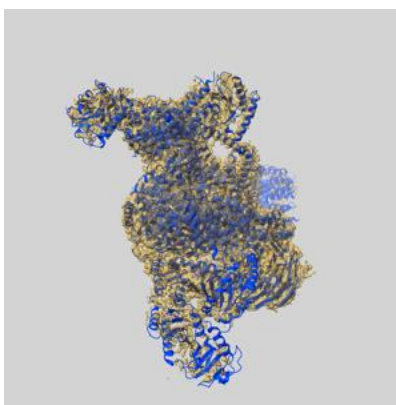
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26857 and PDB model 7UXC. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

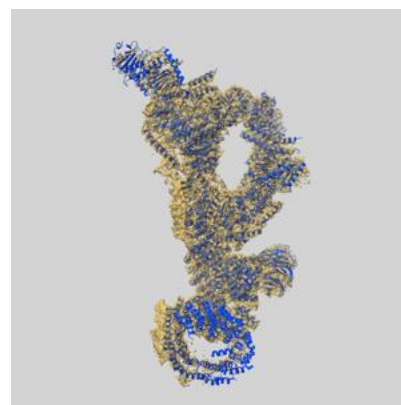
### 9.1 Map-model overlay [i](#)



X



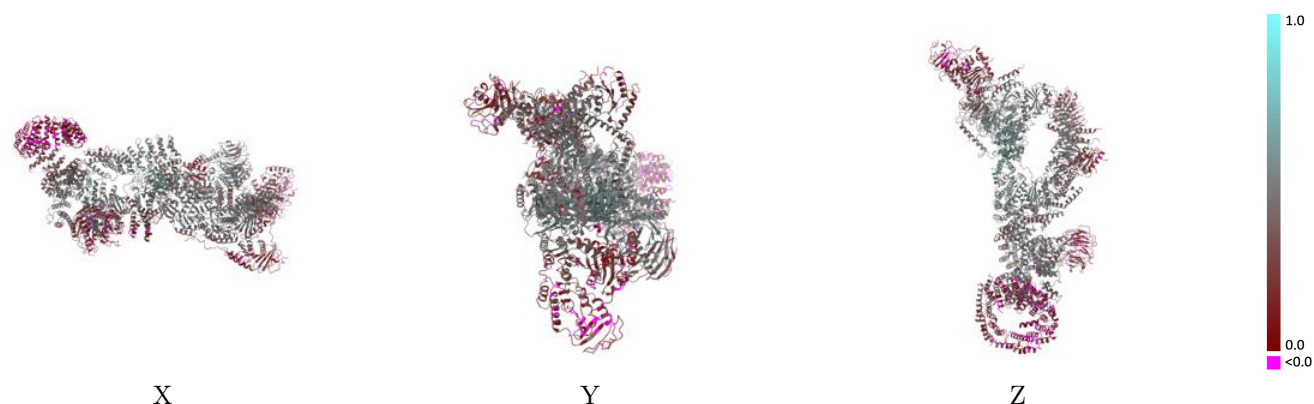
Y



Z

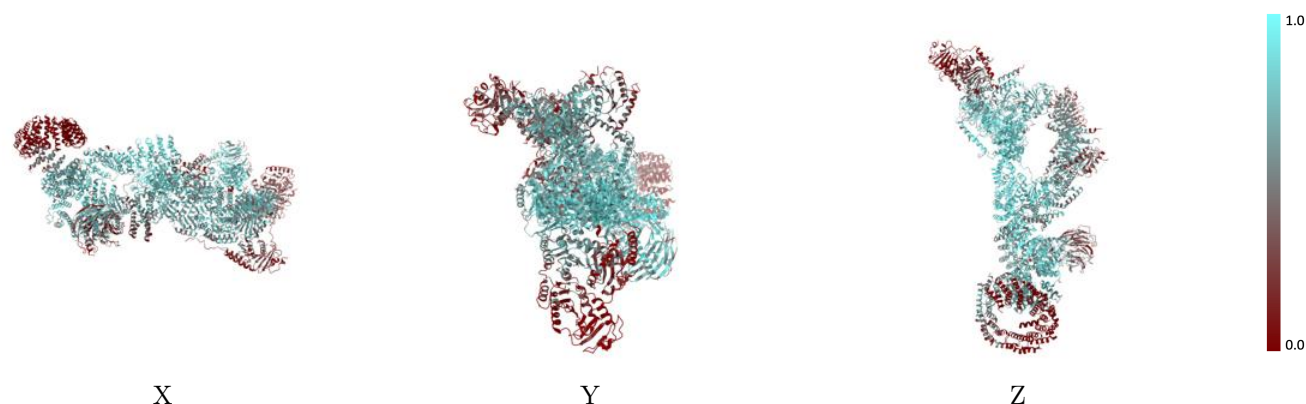
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



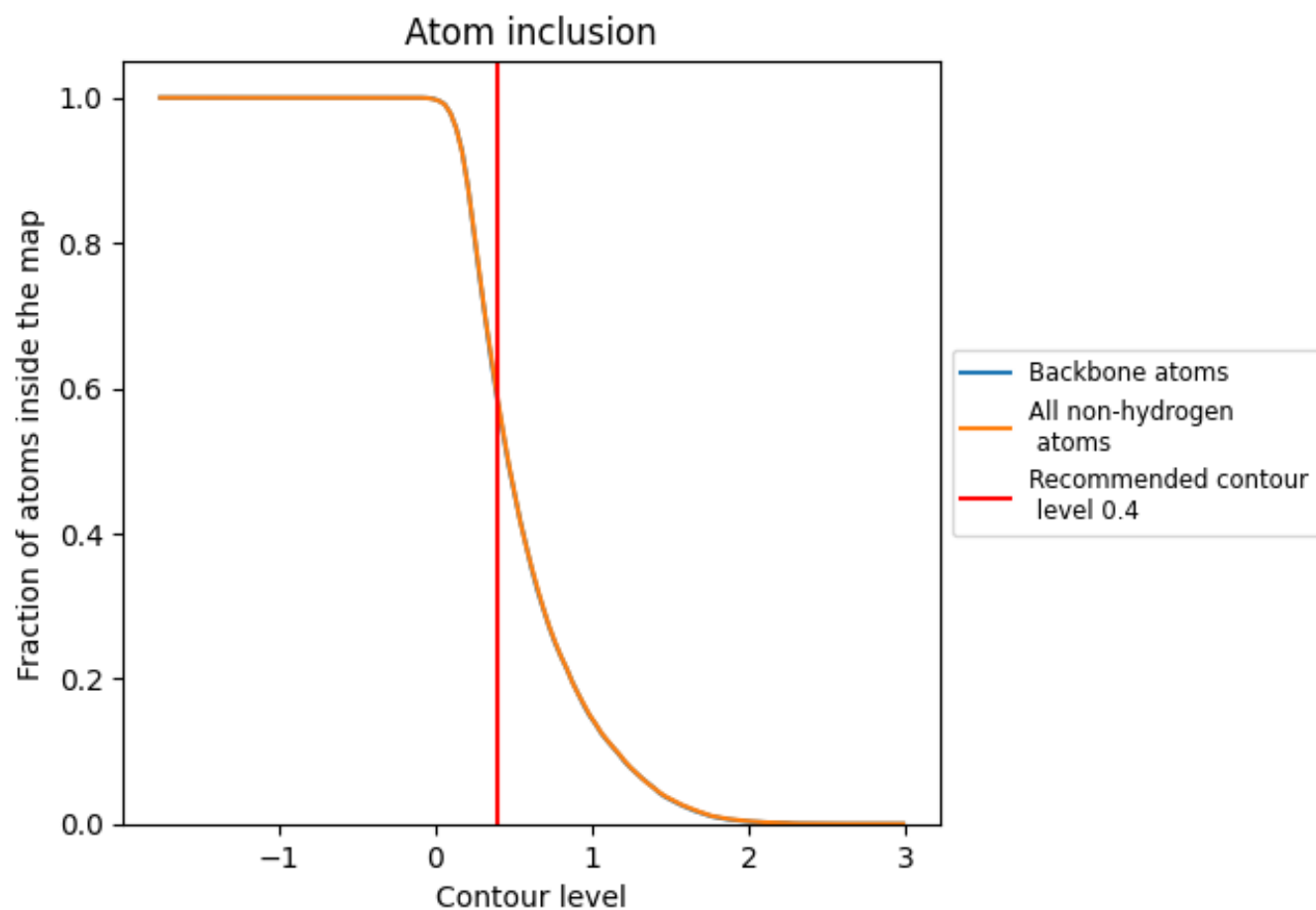
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 58% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5837	 0.3750
A	 0.5806	 0.3560
B	 0.3502	 0.1940
C	 0.8099	 0.4940
D	 0.8030	 0.4950
E	 0.7341	 0.4590
F	 0.1880	 0.1880
G	 0.4816	 0.3070
H	 0.2978	 0.2360
I	 0.0350	 0.1180
J	 0.1470	 0.1810
K	 0.6550	 0.4260
L	 0.5221	 0.3620
M	 0.3132	 0.2710
N	 0.5727	 0.3930
O	 0.5815	 0.3820
P	 0.2083	 0.2050
Q	 0.2665	 0.2480
R	 0.6088	 0.4140

