



Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 10:13 pm GMT

PDB ID : 6SB0
EMDB ID : EMD-10132
Title : cryo-EM structure of mTORC1 bound to PRAS40-fused active RagA/C GT-Pases
Authors : Anandapadamanaban, M.; Berndt, A.; Masson, G.R.; Perisic, O.; Williams, R.L.
Deposited on : 2019-07-18
Resolution : 5.50 Å (reported)
Based on initial models : 6BCX, 6S6A

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

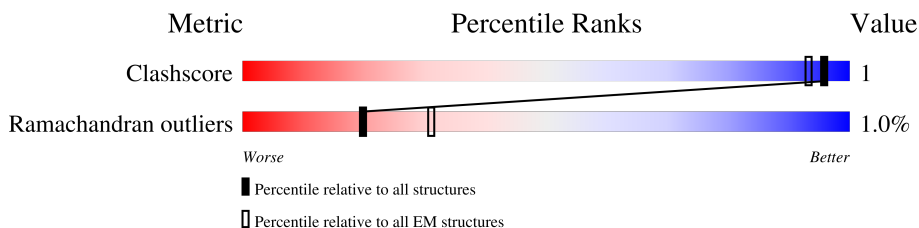
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 5.50 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.



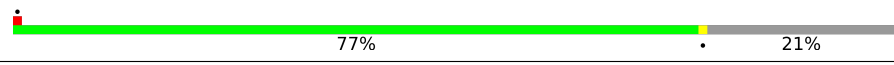


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	2549	
1	B	2549	
2	E	326	
2	H	326	
3	C	313	
3	I	313	
4	D	399	
4	J	399	
5	N	1335	

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Mol	Chain	Length	Quality of chain
5	Y	1335	 77% 21%
6	O	256	 11% 86%
6	T	256	 11% 86%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 41284 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 mTOR,Serine/threonine-protein kinase mTOR,mTOR,Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	2178	10799	6443	2178	2178	0	0
1	B	2178	10799	6443	2178	2178	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	E	317	1562	928	317	317	0	0
2	H	317	1562	928	317	317	0	0

- Molecule 3 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	298	1483	887	298	298	0	0
3	I	298	1482	886	298	298	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	66	LEU	GLN	engineered mutation	UNP Q7L523
I	66	LEU	GLN	engineered mutation	UNP Q7L523

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	272	1349	805	272	272	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	J	273	1354	808	273	273	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	90	ASN	THR	engineered mutation	UNP Q9HB90
J	90	ASN	THR	engineered mutation	UNP Q9HB90

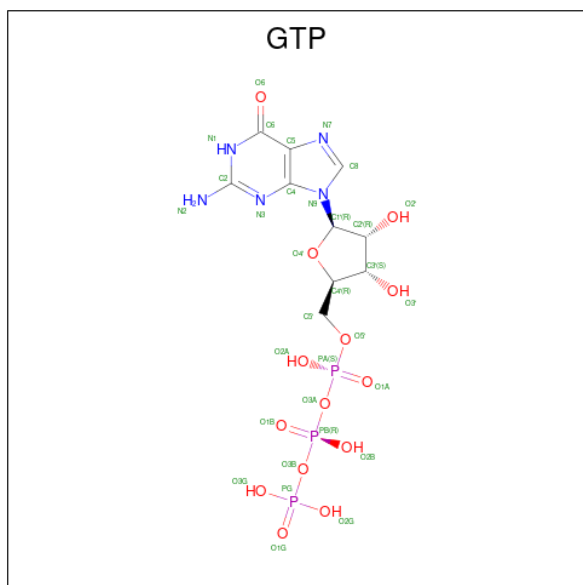
- Molecule 5 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	Y	1052	5214	3110	1052	1052	0	0
5	N	1052	5214	3110	1052	1052	0	0

- Molecule 6 is a protein called Proline-rich AKT1 substrate 1.

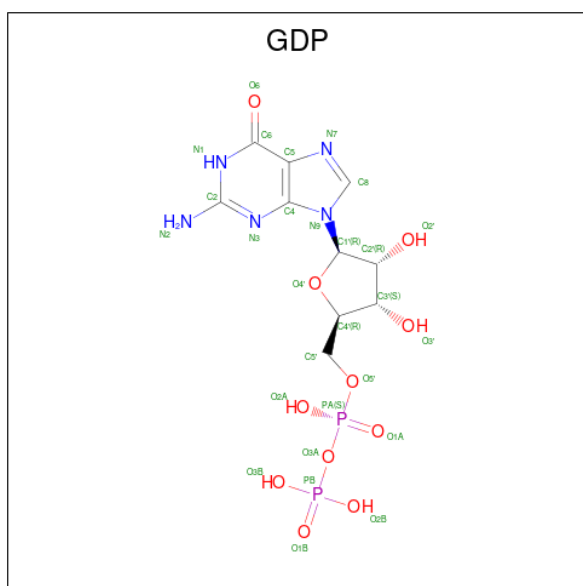
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	T	35	173	103	35	35	0	0
6	O	35	173	103	35	35	0	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
7	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	I	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
8	D	1	Total	C	N	O	P	0
			28	10	5	11	2	

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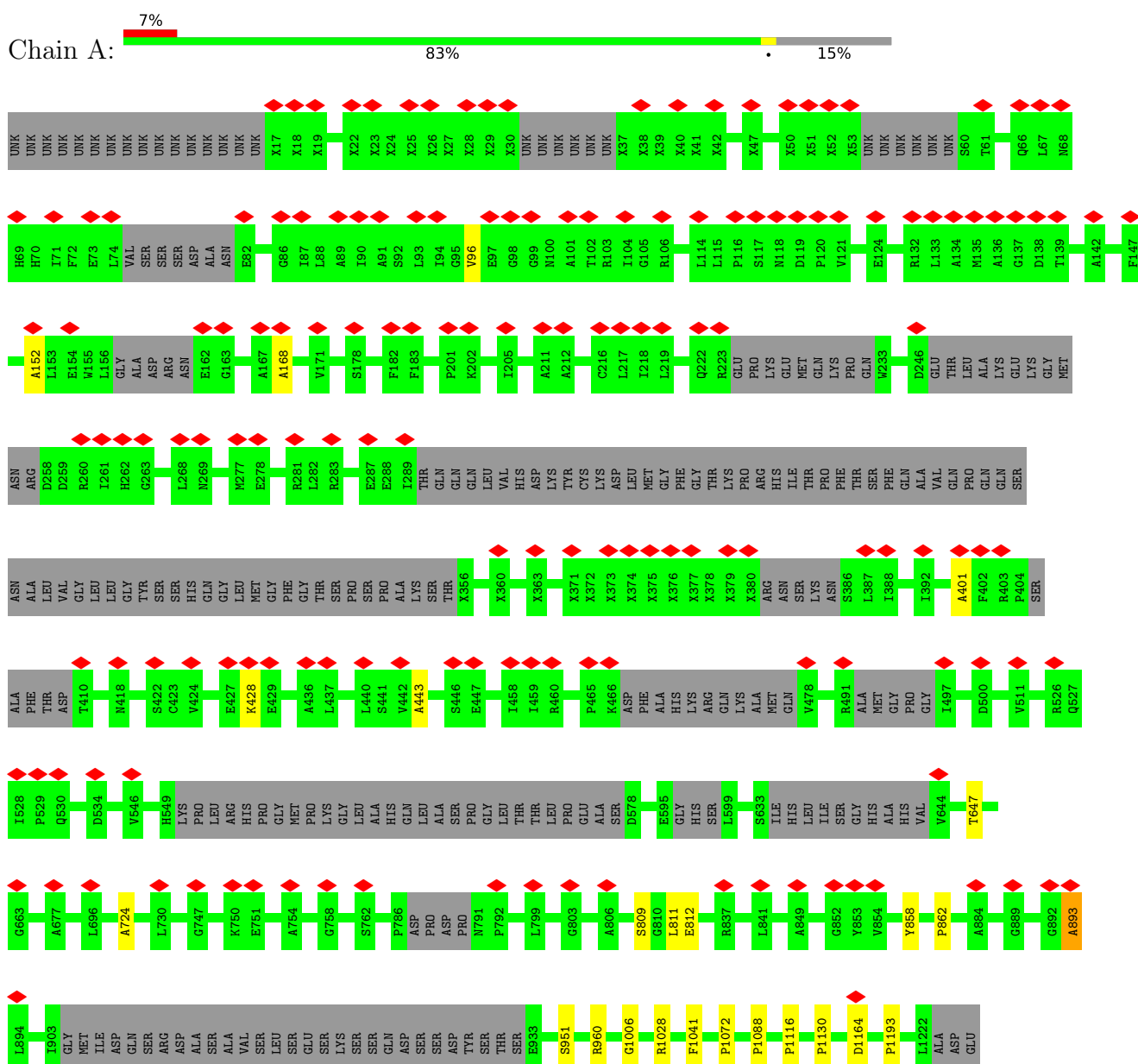
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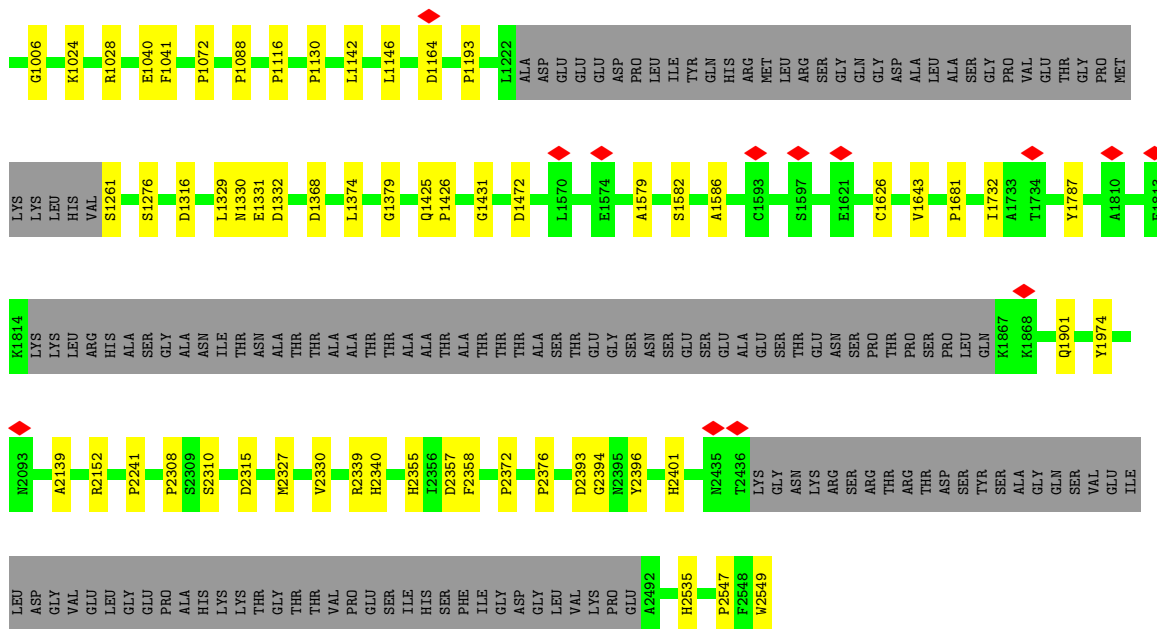
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	J	1	28	10	5	11	2	0

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: mTOR,Serine/threonine-protein kinase mTOR,mTOR,Serine/threonine-protein kinase mTOR





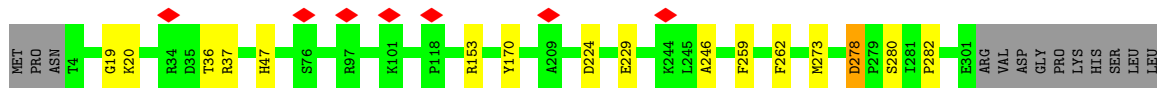
• Molecule 2: Target of rapamycin complex subunit LST8



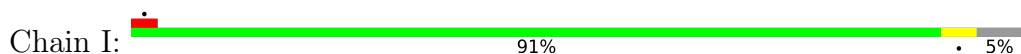
• Molecule 2: Target of rapamycin complex subunit LST8

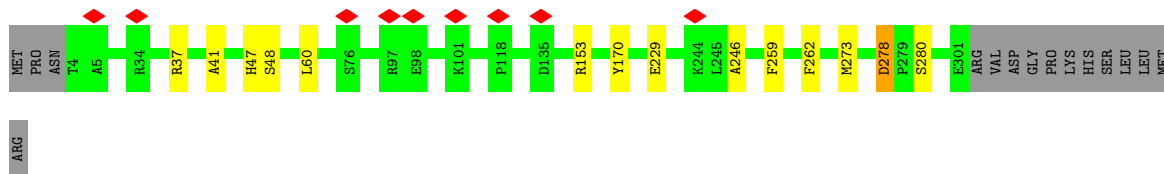


• Molecule 3: Ras-related GTP-binding protein A

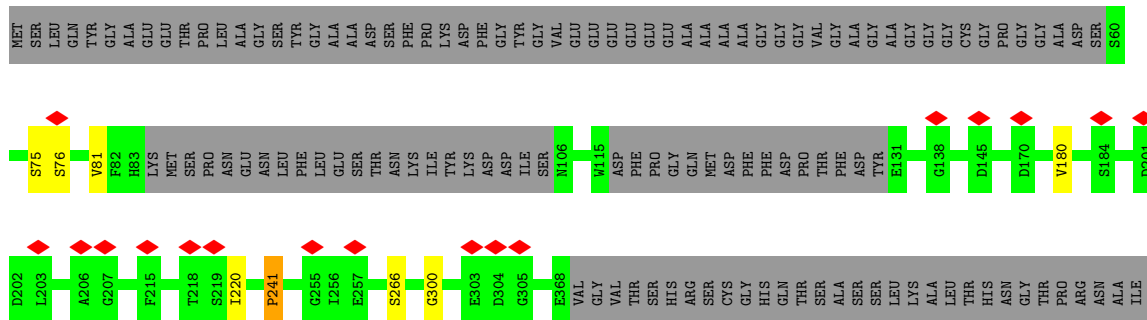


• Molecule 3: Ras-related GTP-binding protein A

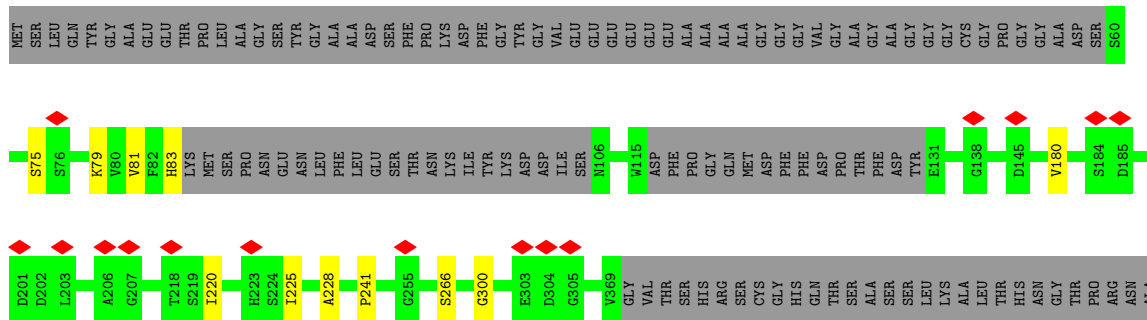




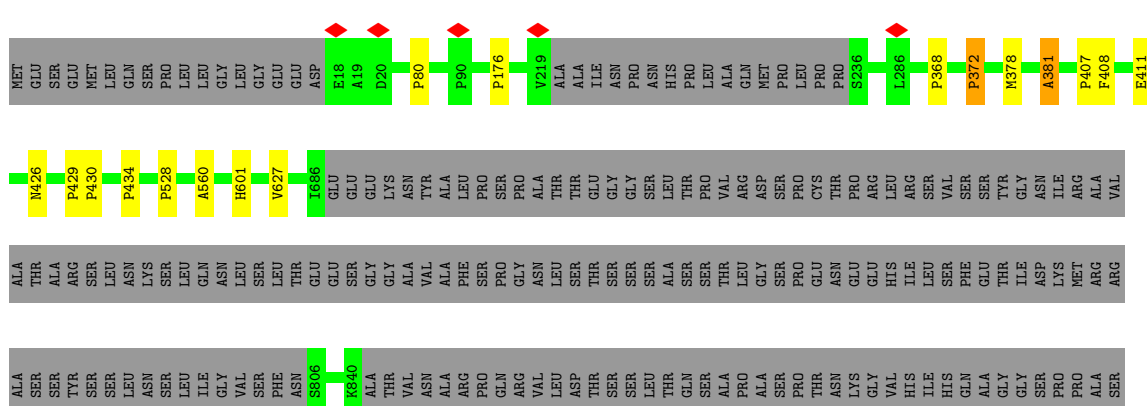
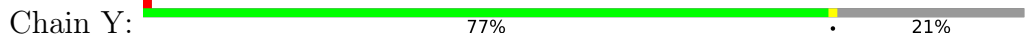
● Molecule 4: Ras-related GTP-binding protein C

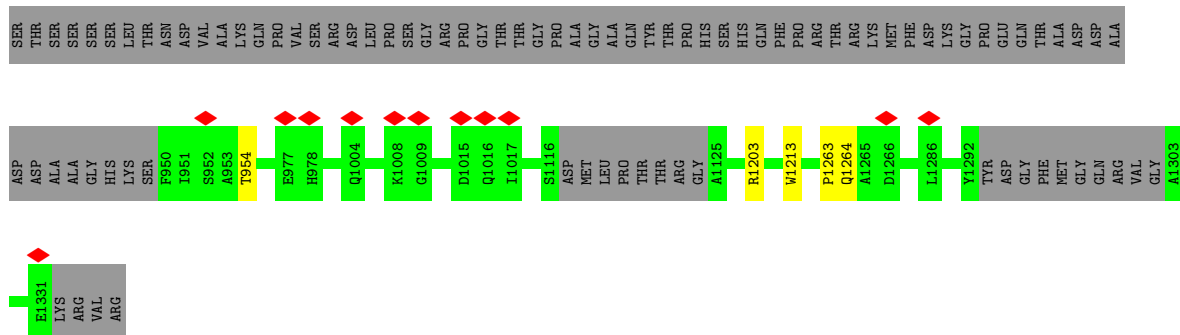


● Molecule 4: Ras-related GTP-binding protein C

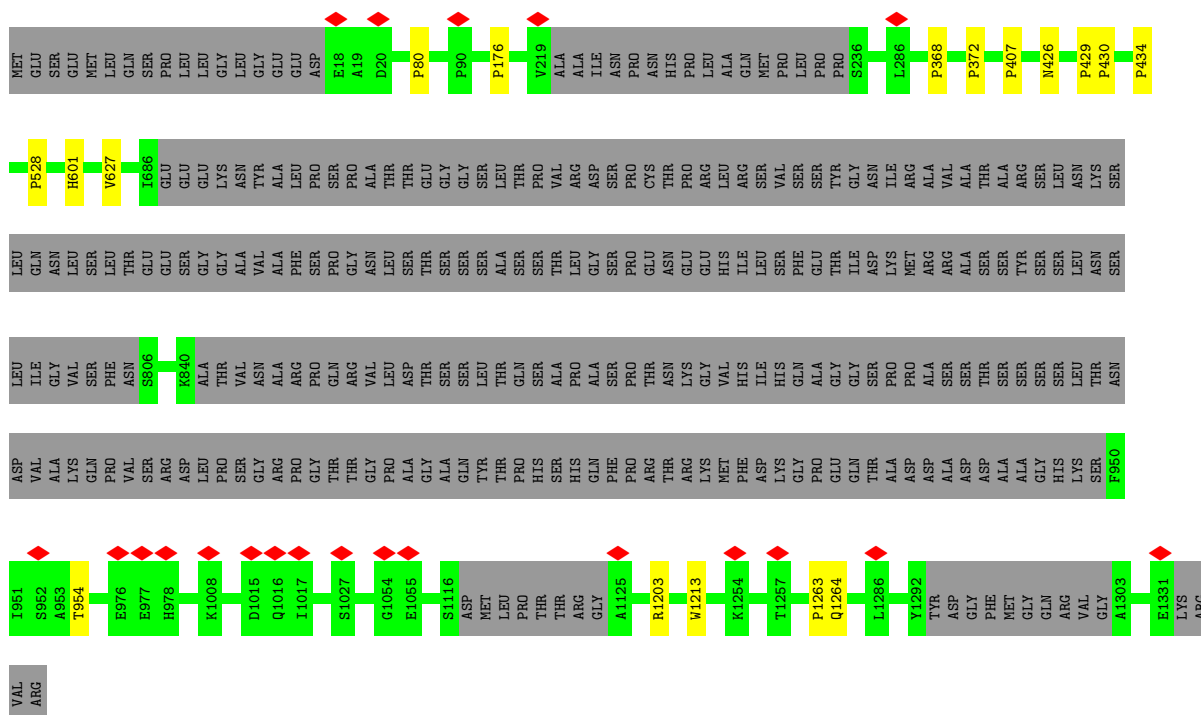
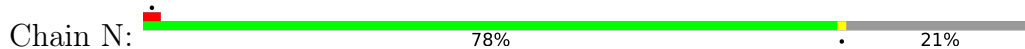


● Molecule 5: Regulatory-associated protein of mTOR

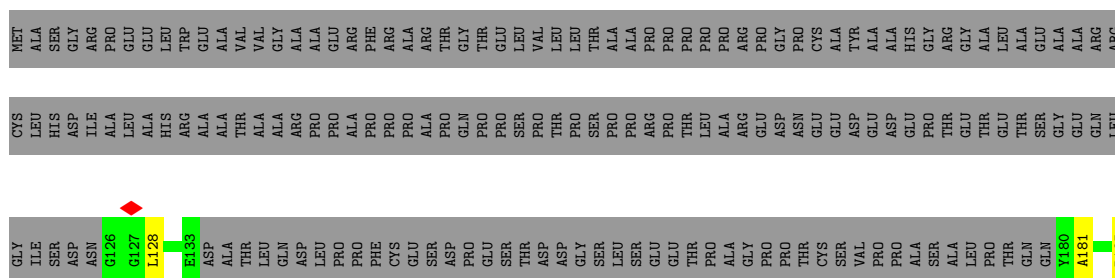




• Molecule 5: Regulatory-associated protein of mTOR



• Molecule 6: Proline-rich AKT1 substrate 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90809	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 ($e^-/\text{\AA}^2$)	40	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	0.118	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	500.49997, 500.49997, 500.49997	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	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: GDP, GTP

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	0.52	2/10502 (0.0%)	0.93	20/14621 (0.1%)
1	B	0.55	1/10502 (0.0%)	1.02	31/14621 (0.2%)
2	E	0.50	0/1561	1.01	1/2170 (0.0%)
2	H	0.48	0/1561	0.97	1/2170 (0.0%)
3	C	0.48	0/1482	0.99	2/2069 (0.1%)
3	I	0.48	0/1481	0.97	0/2067
4	D	0.57	0/1346	0.99	1/1873 (0.1%)
4	J	0.57	0/1351	0.99	0/1880
5	N	0.51	0/5208	0.98	5/7254 (0.1%)
5	Y	0.54	0/5208	1.05	7/7254 (0.1%)
6	O	0.59	0/170	1.23	1/232 (0.4%)
6	T	0.59	0/170	1.27	1/232 (0.4%)
All	All	0.53	3/40542 (0.0%)	0.99	70/56443 (0.1%)

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
1	A	0	5
1	B	0	6
2	E	0	2
2	H	0	2
5	N	0	2
5	Y	0	3
All	All	0	20

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2549	TRP	C-O	7.79	1.38	1.23
1	A	2549	TRP	C-O	5.97	1.34	1.23
1	A	951	SER	CA-CB	-5.31	1.45	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	434	PRO	N-CA-CB	-13.42	87.19	103.30
1	B	1426	PRO	N-CA-CB	-11.71	89.24	103.30
1	B	1681	PRO	N-CA-CB	11.24	116.78	103.30
1	A	1681	PRO	N-CA-CB	10.67	116.11	103.30
5	N	434	PRO	N-CA-CB	-9.89	91.44	103.30
1	B	1072	PRO	N-CA-CB	-9.39	92.03	103.30
1	B	2376	PRO	N-CA-CB	8.73	113.78	103.30
5	Y	426	ASN	CB-CA-C	8.19	126.78	110.40
5	N	426	ASN	CB-CA-C	8.17	126.75	110.40
5	Y	407	PRO	N-CA-CB	-8.17	93.50	103.30
1	A	2376	PRO	N-CA-CB	8.08	113.00	103.30
1	A	1426	PRO	N-CA-CB	-8.07	93.62	103.30
5	Y	368	PRO	N-CA-CB	-7.90	93.82	103.30
1	A	2358	PHE	CB-CA-C	7.50	125.40	110.40
1	B	1130	PRO	N-CA-CB	-7.46	94.35	103.30
1	B	2358	PHE	CB-CA-C	7.46	125.32	110.40
1	B	2310	SER	N-CA-CB	-7.45	99.32	110.50
1	B	1041	PHE	CB-CA-C	7.33	125.06	110.40
6	O	185	PRO	N-CA-CB	7.25	112.01	103.30
6	T	185	PRO	N-CA-CB	7.17	111.91	103.30
1	B	1193	PRO	N-CA-CB	-7.11	94.76	103.30
1	A	1041	PHE	CB-CA-C	7.03	124.45	110.40
1	B	2372	PRO	N-CA-CB	6.75	111.40	103.30
1	A	2372	PRO	N-CA-CB	6.62	111.24	103.30
5	N	368	PRO	N-CA-CB	-6.48	95.47	102.60
1	A	2393	ASP	CB-CA-C	6.47	123.34	110.40
1	A	2547	PRO	N-CA-CB	6.42	111.00	103.30
1	A	1072	PRO	N-CA-CB	-6.35	95.61	102.60
1	B	960	ARG	CB-CA-C	6.31	123.02	110.40
1	A	2241	PRO	CB-CA-C	-6.24	96.40	112.00
1	B	2241	PRO	CB-CA-C	-6.19	96.53	112.00
1	B	2547	PRO	N-CA-CB	6.03	110.53	103.30
1	B	2355	HIS	CB-CA-C	6.02	122.45	110.40
1	B	2315	ASP	CB-CA-C	-6.02	98.36	110.40
1	B	1974	TYR	CB-CA-C	5.89	122.19	110.40
5	Y	429	PRO	CB-CA-C	-5.86	97.35	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	408	PHE	CB-CA-C	-5.86	98.69	110.40
1	B	2357	ASP	CB-CA-C	-5.85	98.70	110.40
1	B	2393	ASP	CB-CA-C	5.81	122.01	110.40
1	A	1974	TYR	CB-CA-C	5.76	121.93	110.40
2	E	195	TYR	CB-CA-C	5.65	121.70	110.40
1	B	1040	GLU	CB-CA-C	-5.61	99.18	110.40
1	B	2396	TYR	N-CA-CB	5.60	120.67	110.60
1	A	2310	SER	N-CA-CB	-5.58	102.14	110.50
1	A	1193	PRO	N-CA-CB	-5.51	96.53	102.60
5	N	407	PRO	N-CA-CB	-5.48	96.57	102.60
1	B	1787	TYR	N-CA-CB	5.45	120.41	110.60
1	A	960	ARG	CB-CA-C	5.43	121.27	110.40
1	B	1901	GLN	CA-C-N	-5.38	105.36	117.20
3	C	282	PRO	N-CA-CB	5.36	109.73	103.30
5	Y	372	PRO	CB-CA-C	-5.36	98.61	112.00
2	H	195	TYR	CB-CA-C	5.35	121.11	110.40
1	B	1024	LYS	CB-CA-C	5.33	121.06	110.40
1	A	1130	PRO	N-CA-CB	-5.33	96.74	102.60
5	N	429	PRO	CB-CA-C	-5.33	98.68	112.00
1	B	2401	HIS	CB-CA-C	5.29	120.98	110.40
4	D	241	PRO	N-CA-CB	5.29	109.65	103.30
1	A	1373	PRO	N-CA-CB	-5.28	96.80	102.60
1	B	1368	ASP	CB-CA-C	5.22	120.85	110.40
1	B	1116	PRO	N-CA-CB	-5.19	96.89	102.60
1	B	960	ARG	C-N-CA	5.12	134.49	121.70
1	B	2339	ARG	CB-CA-C	5.10	120.59	110.40
1	A	2262	ASN	CB-CA-C	5.09	120.59	110.40
1	B	1316	ASP	CB-CA-C	5.08	120.57	110.40
1	B	2535	HIS	CB-CA-C	5.08	120.55	110.40
3	C	224	ASP	CB-CA-C	5.07	120.54	110.40
1	A	2355	HIS	CB-CA-C	5.03	120.46	110.40
1	A	2400	CYS	CB-CA-C	-5.02	100.35	110.40
1	A	1368	ASP	CB-CA-C	5.02	120.44	110.40
1	B	1787	TYR	CB-CA-C	-5.00	100.39	110.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1164	ASP	Peptide
1	A	1261	SER	Peptide
1	A	1732	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	A	1898	ASN	Peptide
1	A	2340	HIS	Peptide
1	B	1164	ASP	Peptide
1	B	1261	SER	Peptide
1	B	1329	LEU	Peptide
1	B	1425	GLN	Peptide
1	B	1732	ILE	Peptide
1	B	2340	HIS	Peptide
2	E	267	GLU	Peptide
2	E	28	GLN	Peptide
2	H	267	GLU	Peptide
2	H	28	GLN	Peptide
5	N	430	PRO	Peptide
5	N	627	VAL	Peptide
5	Y	381	ALA	Mainchain
5	Y	430	PRO	Peptide
5	Y	627	VAL	Peptide

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	10799	0	4791	10	0
1	B	10799	0	4791	11	0
2	E	1562	0	718	0	0
2	H	1562	0	718	0	0
3	C	1483	0	651	11	0
3	I	1482	0	647	10	0
4	D	1349	0	589	4	0
4	J	1354	0	591	5	0
5	N	5214	0	2322	1	0
5	Y	5214	0	2322	5	0
6	O	173	0	82	2	0
6	T	173	0	82	2	0
7	C	32	0	12	4	0
7	I	32	0	12	3	0
8	D	28	0	12	3	0
8	J	28	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	41284	0	18352	56	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.

All (56) 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:N:176:PRO:CB	6:O:181:ALA:O	2.19	0.89
3:I:41:ALA:HB1	7:I:401:GTP:O1G	1.73	0.87
5:Y:176:PRO:CB	6:T:181:ALA:O	2.23	0.86
4:D:75:SER:CB	8:D:401:GDP:O3B	2.29	0.81
3:I:37:ARG:HA	7:I:401:GTP:O3'	1.85	0.77
3:I:47:HIS:HA	3:I:60:LEU:O	1.84	0.76
1:A:724:ALA:HB2	5:Y:411:GLU:CB	2.30	0.62
4:J:75:SER:CB	8:J:401:GDP:O3B	2.52	0.57
3:C:259:PHE:HA	3:C:278:ASP:H	1.70	0.56
3:I:259:PHE:HA	3:I:278:ASP:H	1.70	0.56
4:J:81:VAL:O	4:J:266:SER:CB	2.54	0.56
3:C:37:ARG:HA	7:C:401:GTP:O3'	2.06	0.55
1:A:2139:ALA:HA	1:A:2152:ARG:HA	1.89	0.55
6:T:212:SER:C	6:T:214:ASP:H	2.11	0.54
6:O:212:SER:C	6:O:214:ASP:H	2.11	0.54
1:B:2139:ALA:HA	1:B:2152:ARG:HA	1.88	0.54
4:D:81:VAL:O	4:D:266:SER:CB	2.55	0.53
1:A:1431:GLY:HA3	1:A:2394:GLY:HA2	1.91	0.52
1:B:2327:MET:HA	1:B:2330:VAL:CB	2.38	0.52
1:A:858:TYR:O	1:A:862:PRO:HA	2.10	0.52
1:B:1330:ASN:O	1:B:1332:ASP:N	2.43	0.52
3:C:259:PHE:O	3:C:278:ASP:CB	2.58	0.52
1:B:893:ALA:O	1:B:1626:CYS:HA	2.10	0.51
3:I:259:PHE:O	3:I:278:ASP:CB	2.59	0.51
5:Y:378:MET:O	5:Y:381:ALA:HB3	2.11	0.50
1:B:1579:ALA:HA	1:B:1586:ALA:HB2	1.94	0.50
1:A:1330:ASN:O	1:A:1332:ASP:N	2.46	0.49
4:D:76:SER:CB	8:D:401:GDP:O1A	2.60	0.49
1:B:858:TYR:O	1:B:862:PRO:HA	2.14	0.48
3:I:259:PHE:C	3:I:278:ASP:CB	2.83	0.48
3:C:259:PHE:C	3:C:278:ASP:CB	2.83	0.47
1:A:1579:ALA:HA	1:A:1586:ALA:HB2	1.97	0.47
4:D:220:ILE:CB	8:D:401:GDP:C6	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:220:ILE:CB	8:J:401:GDP:C6	2.98	0.46
3:I:170:TYR:CB	3:I:229:GLU:CB	2.94	0.46
3:C:47:HIS:CB	5:Y:560:ALA:CB	2.93	0.46
1:B:1431:GLY:HA3	1:B:2394:GLY:HA2	1.98	0.45
3:I:37:ARG:N	7:I:401:GTP:O2'	2.51	0.44
1:A:1431:GLY:CA	1:A:2394:GLY:HA2	2.47	0.43
3:C:47:HIS:CB	5:Y:560:ALA:HB1	2.48	0.43
3:C:170:TYR:CB	3:C:229:GLU:CB	2.97	0.42
1:B:152:ALA:O	1:B:168:ALA:HB1	2.18	0.42
3:I:48:SER:N	3:I:60:LEU:O	2.52	0.42
1:A:401:ALA:HA	1:A:443:ALA:HB1	2.01	0.42
4:J:225:ILE:O	4:J:228:ALA:HB3	2.20	0.42
3:C:19:GLY:HA2	7:C:401:GTP:H5'	2.02	0.42
4:J:79:LYS:O	4:J:83:HIS:N	2.50	0.41
1:B:401:ALA:HA	1:B:443:ALA:HB1	2.01	0.41
1:B:1142:LEU:O	1:B:1146:LEU:CB	2.69	0.41
3:C:262:PHE:O	3:C:273:MET:HA	2.21	0.41
3:C:20:LYS:H	7:C:401:GTP:PB	2.43	0.41
3:C:36:THR:C	7:C:401:GTP:O2'	2.59	0.41
1:A:152:ALA:O	1:A:168:ALA:HB1	2.21	0.41
3:I:262:PHE:O	3:I:273:MET:HA	2.21	0.41
1:A:893:ALA:O	1:A:1626:CYS:HA	2.21	0.40
1:B:1374:LEU:O	1:B:1379:GLY:N	2.53	0.40

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%)	1951 (93%)	121 (6%)	16 (1%)	19 59
1	B	2088/2549 (82%)	1949 (93%)	124 (6%)	15 (1%)	22 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	315/326 (97%)	274 (87%)	36 (11%)	5 (2%)	9	43
2	H	315/326 (97%)	270 (86%)	40 (13%)	5 (2%)	9	43
3	C	296/313 (95%)	277 (94%)	15 (5%)	4 (1%)	11	45
3	I	296/313 (95%)	278 (94%)	14 (5%)	4 (1%)	11	45
4	D	266/399 (67%)	242 (91%)	21 (8%)	3 (1%)	14	51
4	J	267/399 (67%)	242 (91%)	22 (8%)	3 (1%)	14	51
5	N	1040/1335 (78%)	932 (90%)	99 (10%)	9 (1%)	17	56
5	Y	1040/1335 (78%)	927 (89%)	104 (10%)	9 (1%)	17	56
6	O	29/256 (11%)	23 (79%)	4 (14%)	2 (7%)	1	14
6	T	29/256 (11%)	23 (79%)	2 (7%)	4 (14%)	0	4
All	All	8069/10356 (78%)	7388 (92%)	602 (8%)	79 (1%)	20	53

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1331	GLU
1	B	1331	GLU
3	C	153	ARG
3	C	280	SER
4	D	180	VAL
3	I	153	ARG
3	I	280	SER
4	J	180	VAL
1	A	647	THR
1	A	1006	GLY
1	A	2308	PRO
1	B	647	THR
1	B	1006	GLY
1	B	1276	SER
1	B	2308	PRO
2	E	118	ASN
2	E	241	ASP
5	Y	601	HIS
5	Y	1213	TRP
2	H	118	ASN
2	H	241	ASP
5	N	1213	TRP
6	O	216	ASP

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Mol	Chain	Res	Type
1	A	893	ALA
1	A	1276	SER
2	E	86	LYS
2	E	87	ASN
2	E	269	SER
3	C	246	ALA
3	C	278	ASP
4	D	300	GLY
5	Y	1203	ARG
6	T	216	ASP
2	H	87	ASN
2	H	269	SER
3	I	278	ASP
5	N	601	HIS
5	N	1203	ARG
1	A	428	LYS
1	A	809	SER
1	A	1088	PRO
1	A	1472	ASP
1	B	428	LYS
1	B	809	SER
1	B	1088	PRO
1	B	1472	ASP
5	Y	80	PRO
5	Y	1264	GLN
2	H	86	LYS
3	I	246	ALA
4	J	300	GLY
5	N	80	PRO
5	N	1264	GLN
1	A	96	VAL
1	A	811	LEU
1	A	1028	ARG
1	B	811	LEU
6	T	213	PRO
6	T	214	ASP
4	J	241	PRO
6	O	213	PRO
1	A	812	GLU
1	A	2357	ASP
1	B	96	VAL
1	B	893	ALA

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Mol	Chain	Res	Type
1	B	1582	SER
4	D	241	PRO
5	Y	528	PRO
5	Y	954	THR
5	Y	1263	PRO
6	T	128	LEU
5	N	954	THR
5	N	1263	PRO
5	Y	372	PRO
5	N	372	PRO
1	B	1028	ARG
1	B	1643	VAL
5	N	528	PRO
1	A	1116	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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$
8	GDP	D	401	-	24,30,30	0.82	1 (4%)	30,47,47	2.03	10 (33%)
7	GTP	C	401	-	26,34,34	1.10	2 (7%)	32,54,54	0.94	1 (3%)
7	GTP	I	401	-	26,34,34	1.22	4 (15%)	32,54,54	1.10	2 (6%)
8	GDP	J	401	-	24,30,30	1.12	3 (12%)	30,47,47	1.88	12 (40%)

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
8	GDP	D	401	-	-	2/12/32/32	0/3/3/3
7	GTP	C	401	-	-	2/18/38/38	0/3/3/3
7	GTP	I	401	-	-	2/18/38/38	0/3/3/3
8	GDP	J	401	-	-	2/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	401	GTP	PG-O1G	-3.32	1.39	1.50
7	C	401	GTP	C5-C6	-2.92	1.41	1.47
7	I	401	GTP	C5-C6	-2.82	1.41	1.47
8	J	401	GDP	O2'-C2'	2.36	1.48	1.43
8	D	401	GDP	C5-C4	2.19	1.48	1.43
8	J	401	GDP	C5-C4	2.17	1.48	1.43
7	C	401	GTP	C8-N7	-2.08	1.31	1.35
7	I	401	GTP	PG-O3G	-2.05	1.46	1.54
7	I	401	GTP	C8-N7	-2.04	1.31	1.35
8	J	401	GDP	C8-N7	2.03	1.38	1.35

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	401	GDP	PA-O3A-PB	-6.02	112.17	132.83
8	J	401	GDP	PA-O3A-PB	-3.86	119.58	132.83
8	D	401	GDP	O3B-PB-O2B	3.79	122.11	107.64
8	D	401	GDP	O6-C6-C5	-3.33	117.86	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	401	GDP	O6-C6-C5	-3.07	118.37	124.37
8	D	401	GDP	C3'-C2'-C1'	2.98	105.47	100.98
8	J	401	GDP	O2B-PB-O1B	2.87	121.92	110.68
8	J	401	GDP	C8-N7-C5	2.79	108.31	102.99
7	I	401	GTP	O3'-C3'-C2'	-2.61	103.39	111.82
8	J	401	GDP	C3'-C2'-C1'	2.57	104.85	100.98
8	D	401	GDP	C5-C6-N1	2.54	118.43	113.95
8	J	401	GDP	O4'-C4'-C5'	-2.53	101.06	109.37
8	D	401	GDP	O6-C6-N1	2.49	123.58	120.65
8	J	401	GDP	C5-C6-N1	2.45	118.29	113.95
8	D	401	GDP	O4'-C4'-C3'	2.36	109.79	105.11
7	I	401	GTP	O3'-C3'-C4'	2.33	117.78	111.05
8	D	401	GDP	O3'-C3'-C2'	-2.26	104.53	111.82
8	J	401	GDP	O3B-PB-O3A	2.22	112.08	104.64
7	C	401	GTP	O3'-C3'-C4'	2.12	117.19	111.05
8	J	401	GDP	O2'-C2'-C3'	2.12	118.69	111.82
8	D	401	GDP	O2'-C2'-C3'	2.12	118.68	111.82
8	D	401	GDP	O3A-PB-O1B	-2.11	99.49	111.19
8	J	401	GDP	O3'-C3'-C2'	-2.09	105.07	111.82
8	J	401	GDP	O3A-PB-O1B	-2.07	99.71	111.19
8	J	401	GDP	O4'-C4'-C3'	2.04	109.15	105.11

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	401	GDP	PA-O3A-PB-O3B
8	J	401	GDP	PA-O3A-PB-O3B
7	C	401	GTP	PA-O3A-PB-O1B
7	C	401	GTP	O4'-C4'-C5'-O5'
8	J	401	GDP	PA-O3A-PB-O1B
8	D	401	GDP	PA-O3A-PB-O2B
7	I	401	GTP	PA-O3A-PB-O1B
7	I	401	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 12 short contacts:

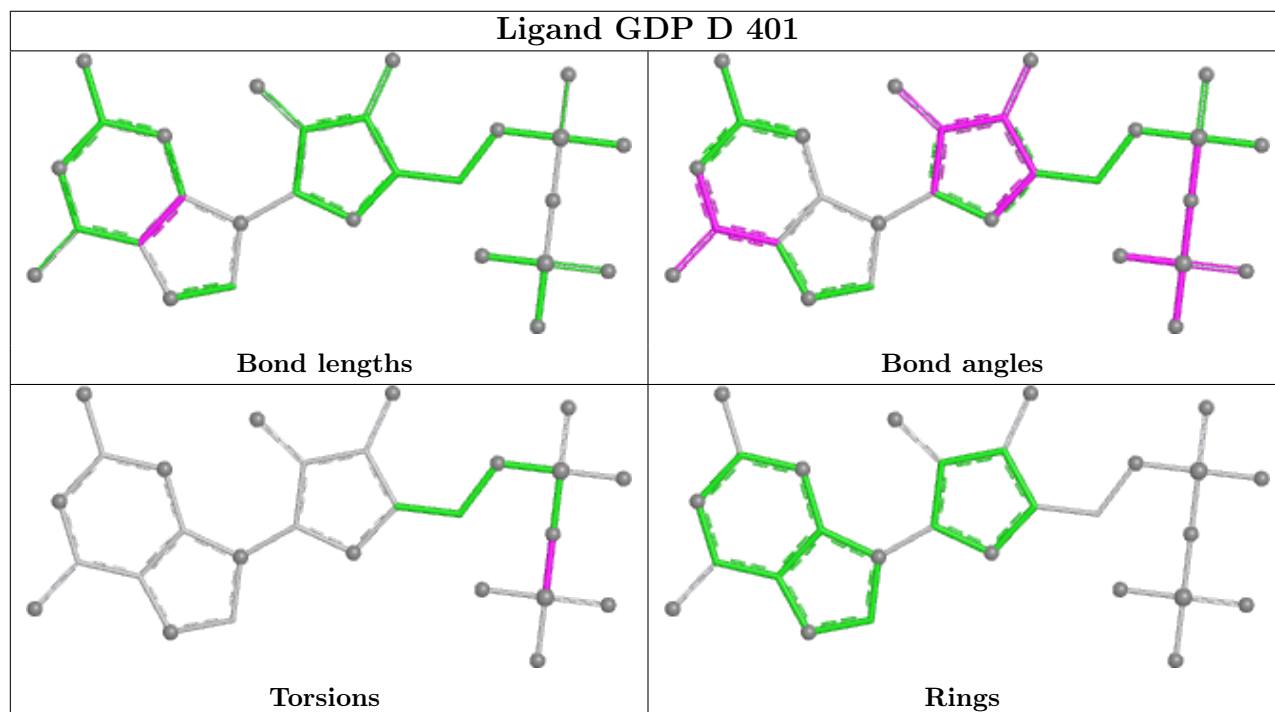
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	401	GDP	3	0
7	C	401	GTP	4	0

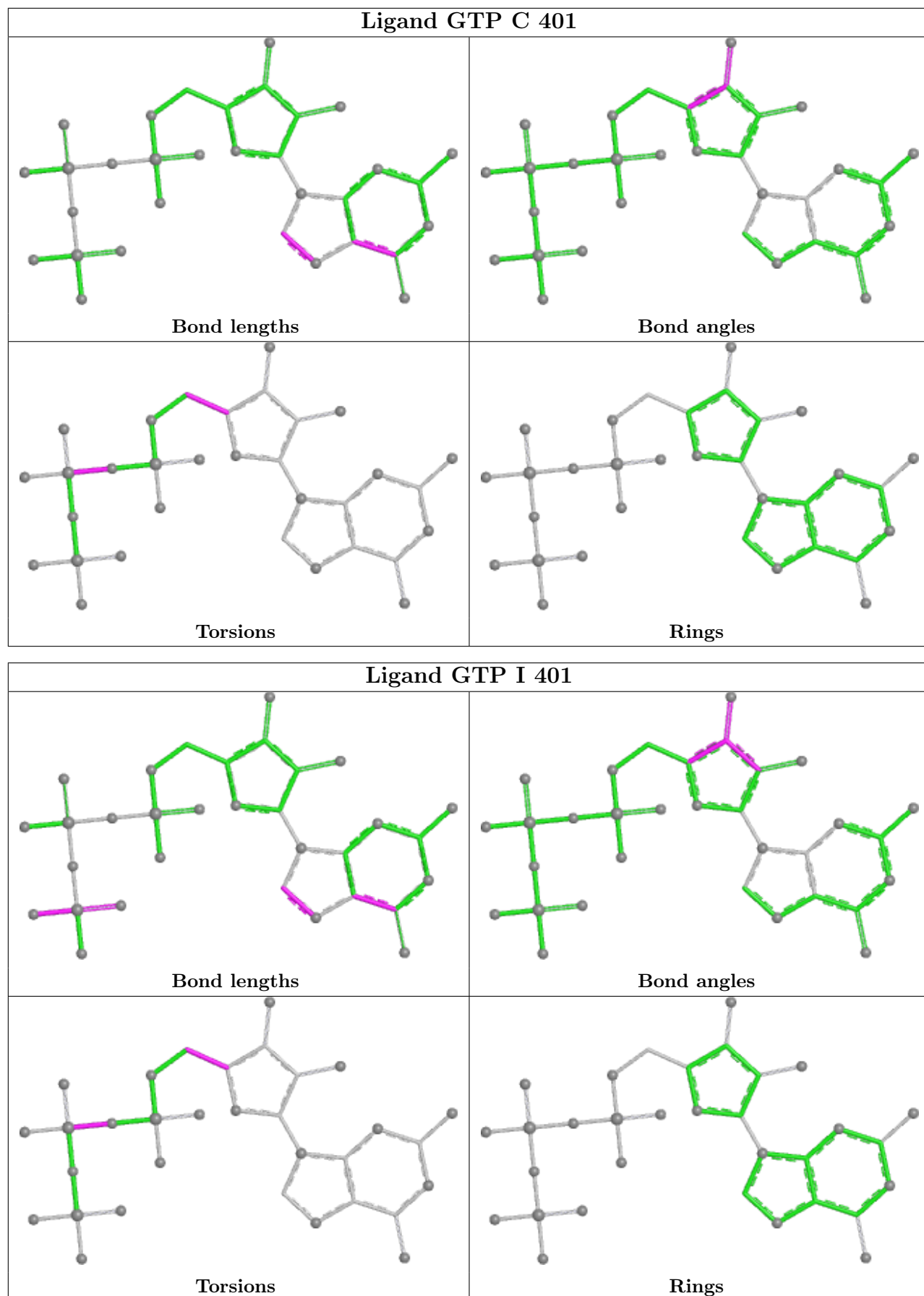
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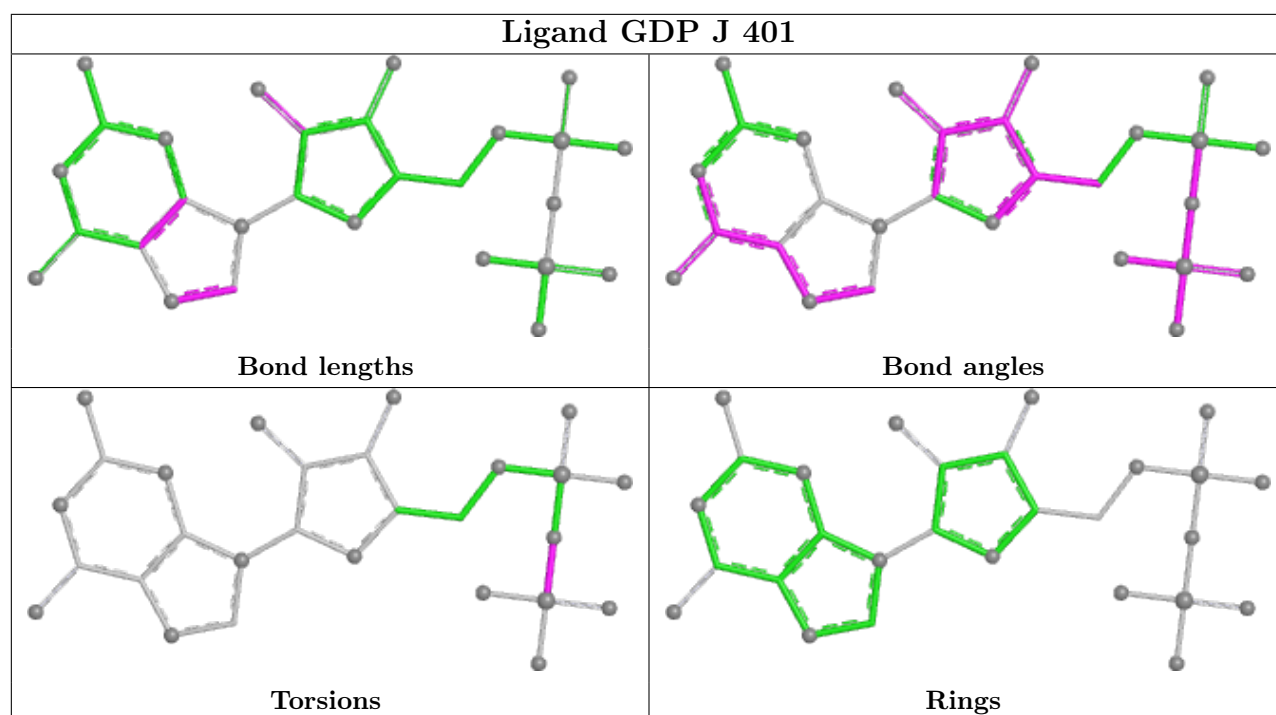
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	401	GTP	3	0
8	J	401	GDP	2	0

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.

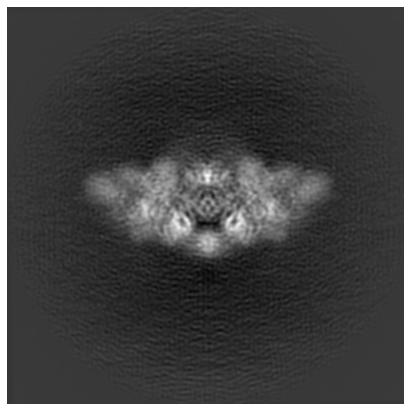
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10132. These allow visual inspection of the internal detail of the map and identification of artifacts.

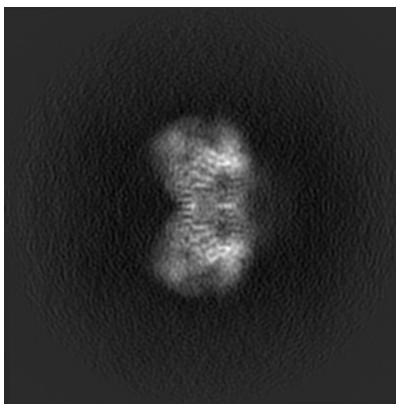
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

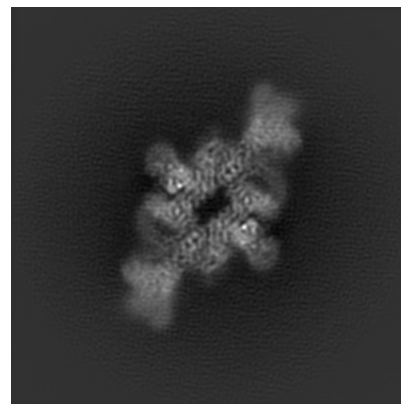
6.1.1 Primary map



X

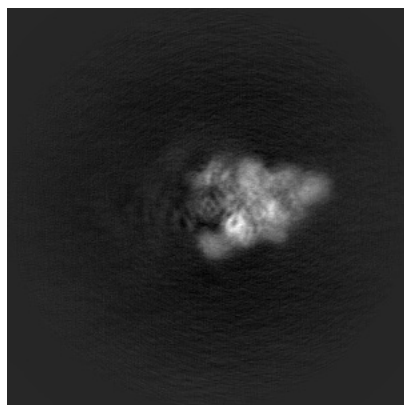


Y

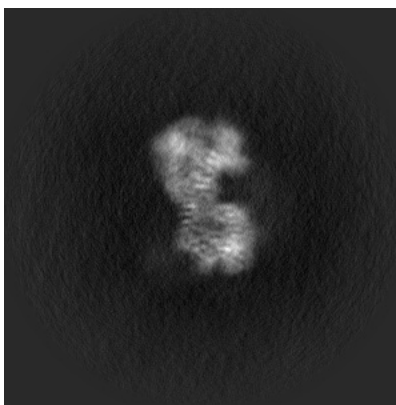


Z

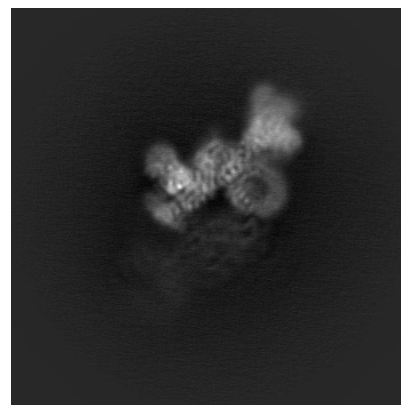
6.1.2 Raw map



X



Y

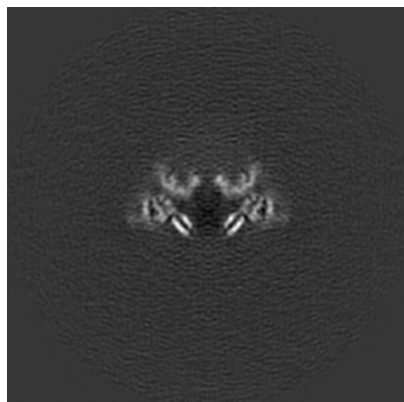


Z

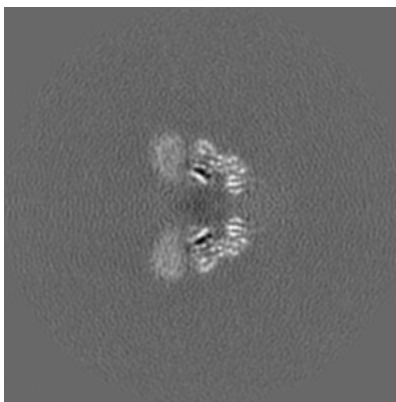
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

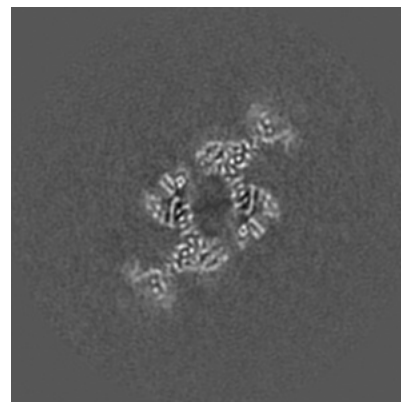
6.2.1 Primary map



X Index: 175

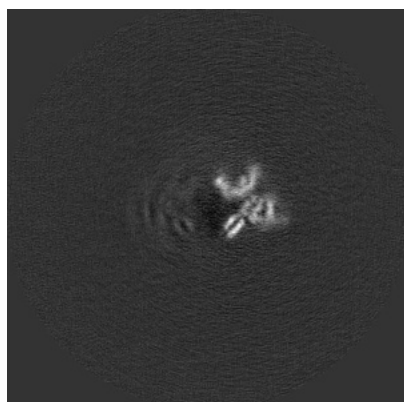


Y Index: 175

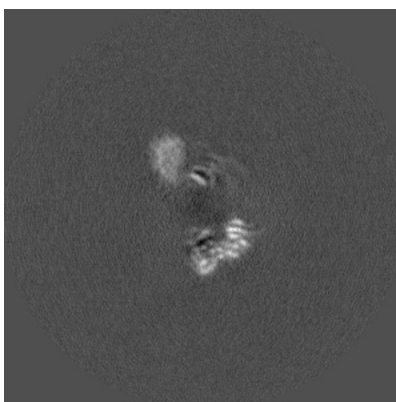


Z Index: 175

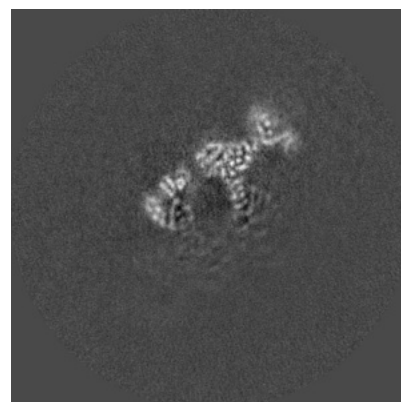
6.2.2 Raw map



X Index: 175



Y Index: 175

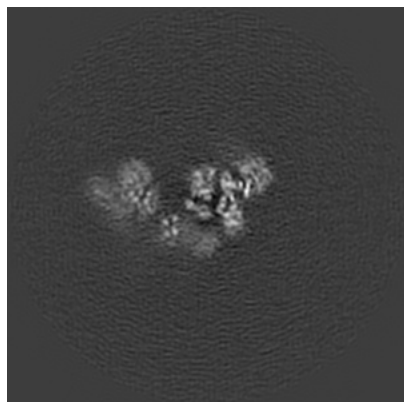


Z Index: 175

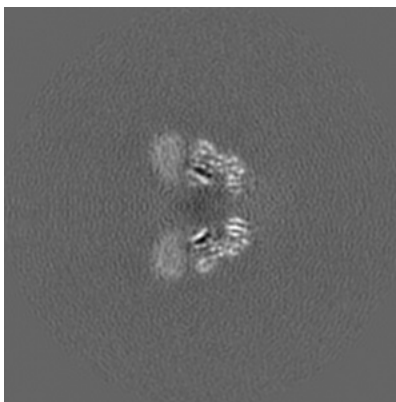
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

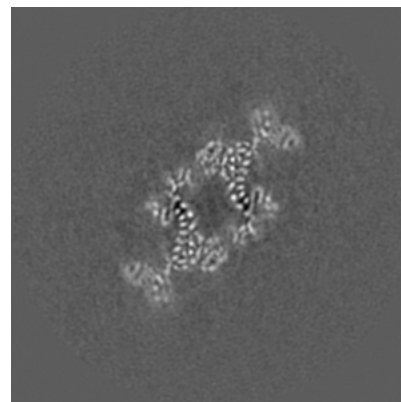
6.3.1 Primary map



X Index: 139

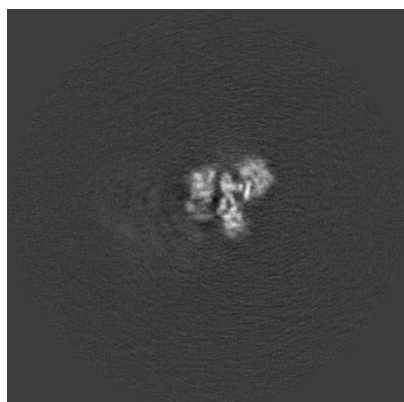


Y Index: 176

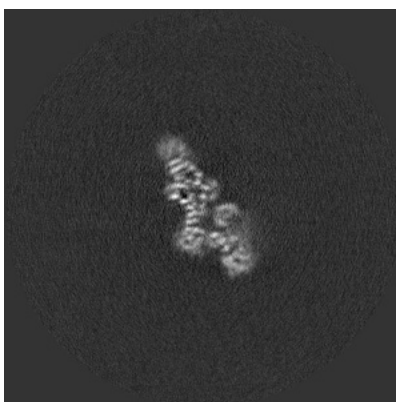


Z Index: 172

6.3.2 Raw map



X Index: 139



Y Index: 205



Z Index: 197

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 0.018. 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.

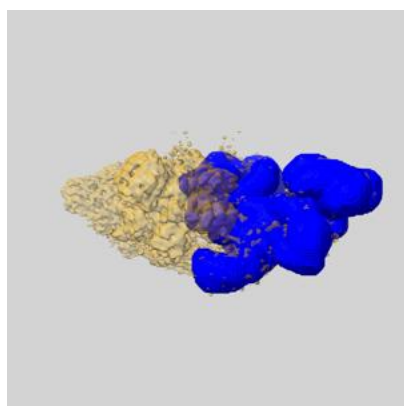
6.5 Mask visualisation [i](#)

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

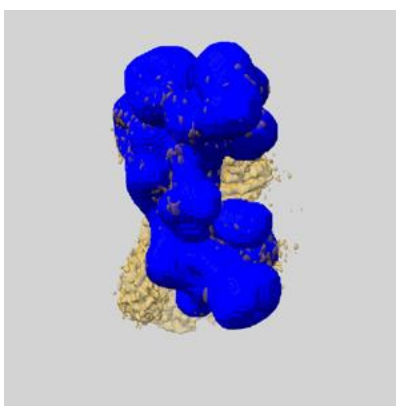
A mask typically either:

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

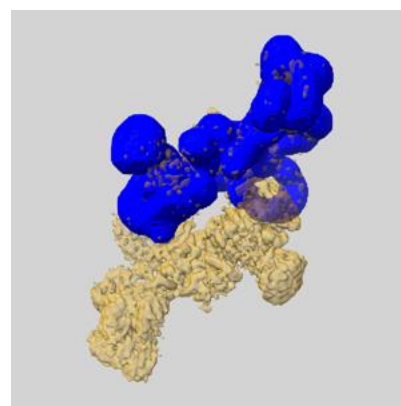
6.5.1 emd_10132_msk_1.map [i](#)



X



Y

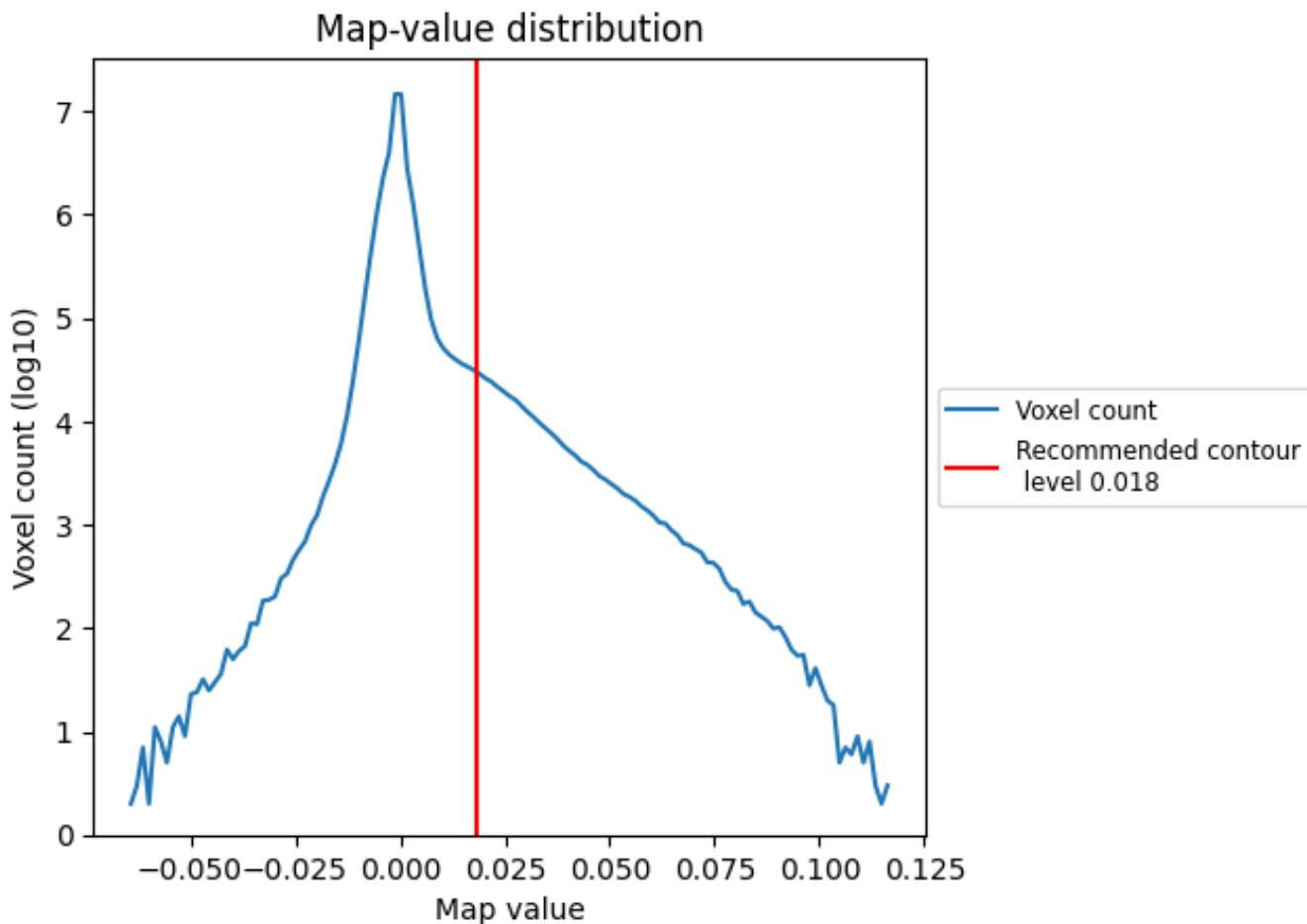


Z

7 Map analysis [i](#)

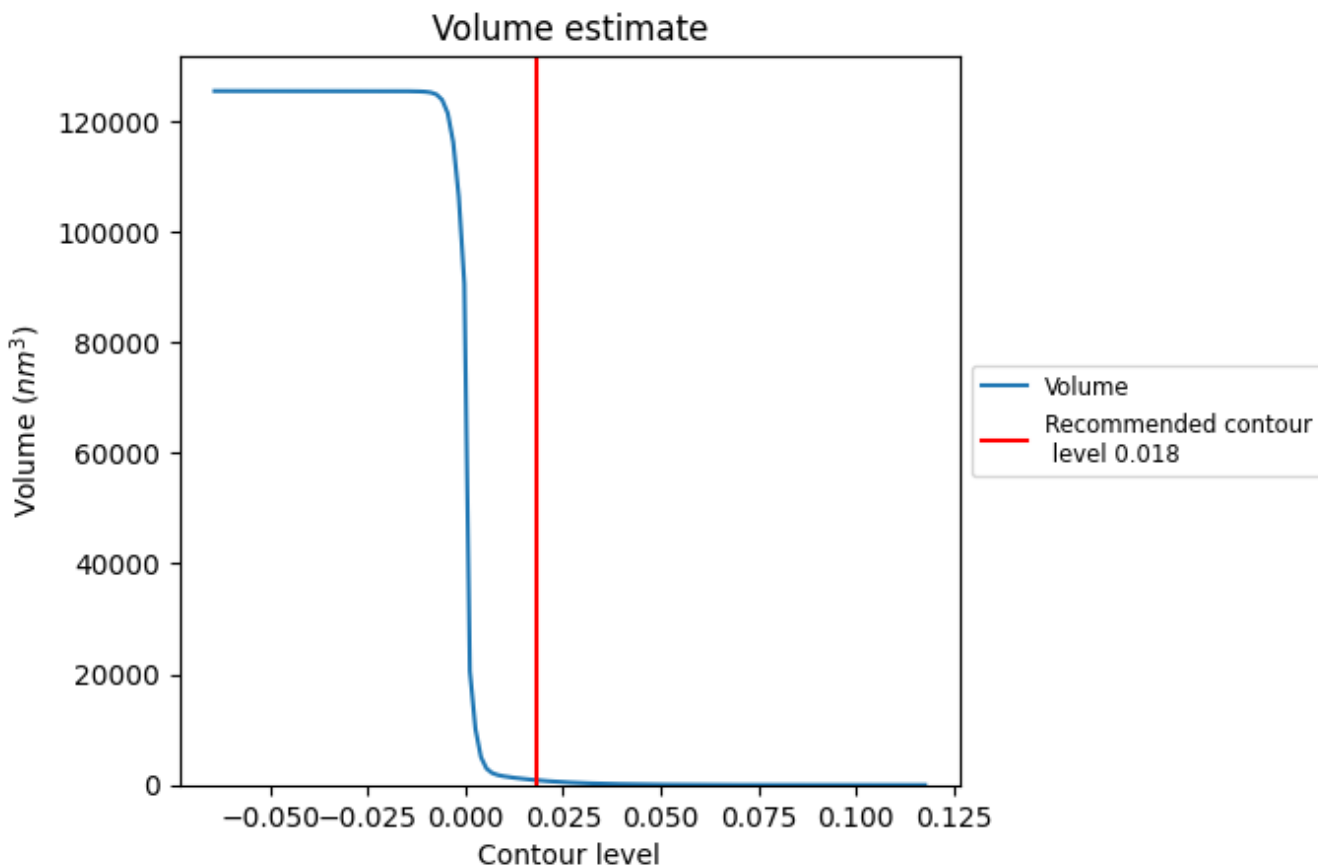
This section contains the results of statistical analysis of the map.

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.

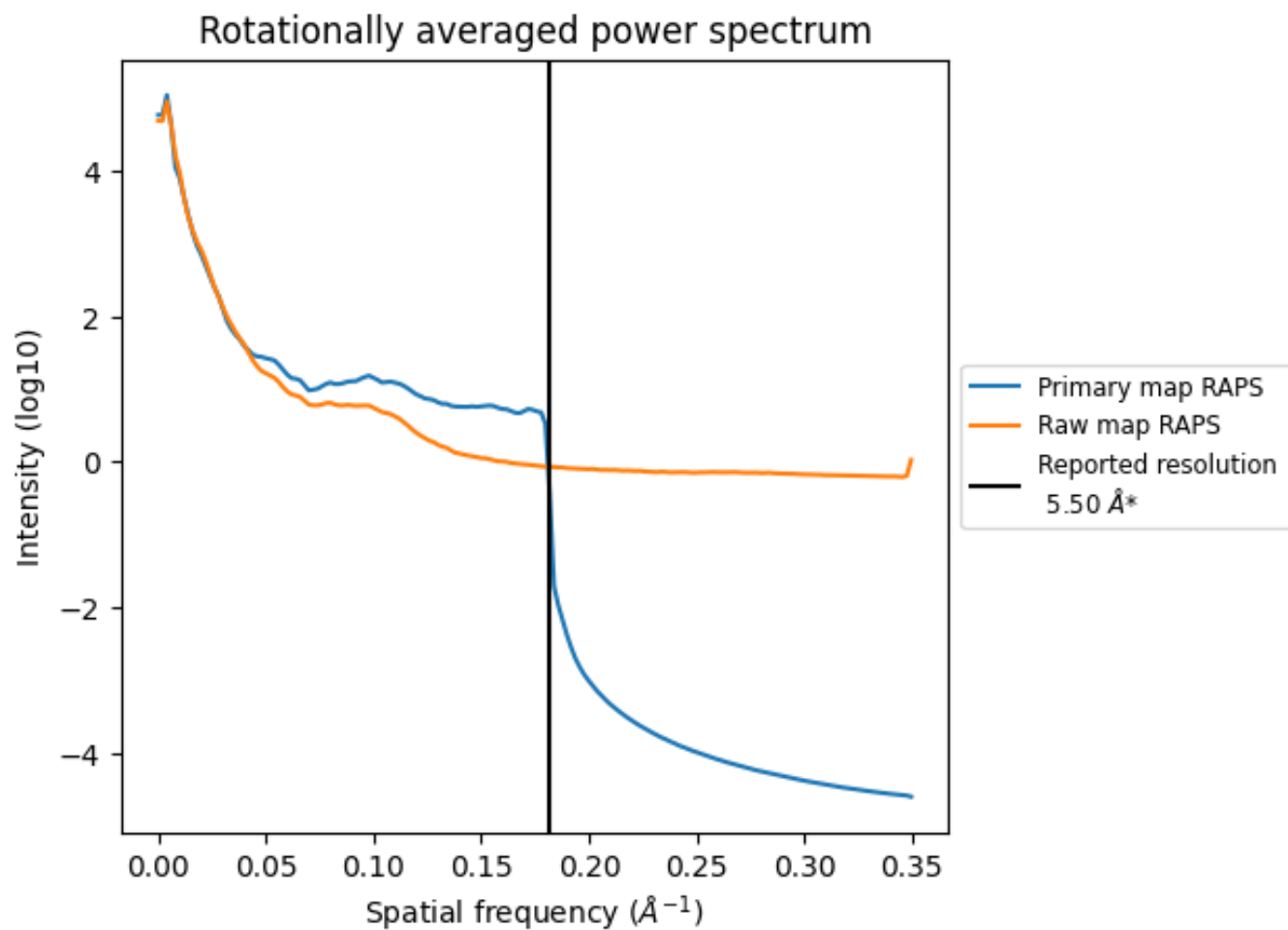
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 880 nm^3 ; this corresponds to an approximate mass of 795 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 [i](#)

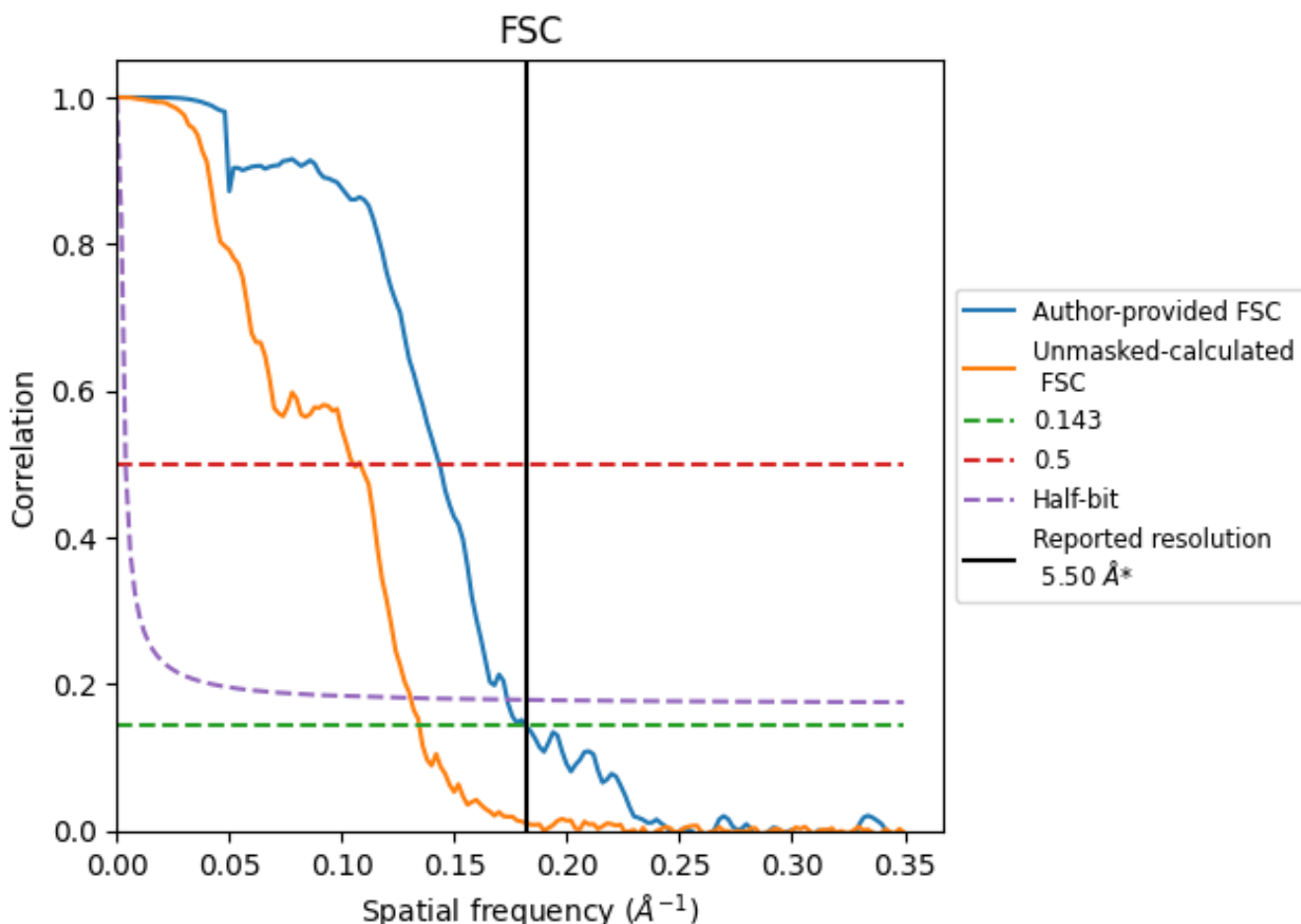


*Reported resolution corresponds to spatial frequency of 0.182 Å⁻¹

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 0.182 Å⁻¹

8.2 Resolution estimates [i](#)

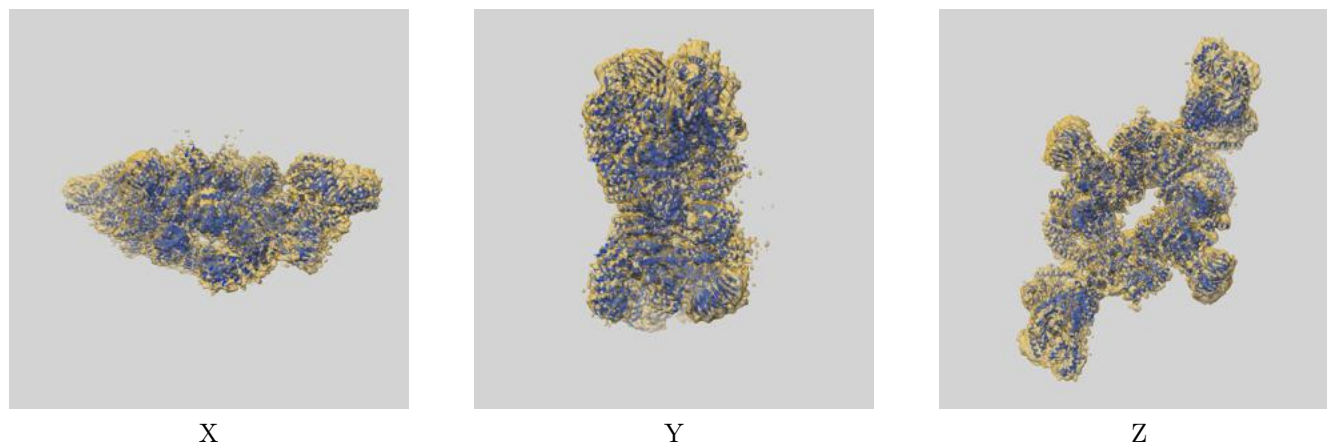
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	5.51	6.98	5.76
Unmasked-calculated*	7.44	9.51	7.66

*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 7.44 differs from the reported value 5.5 by more than 10 %

9 Map-model fit [i](#)

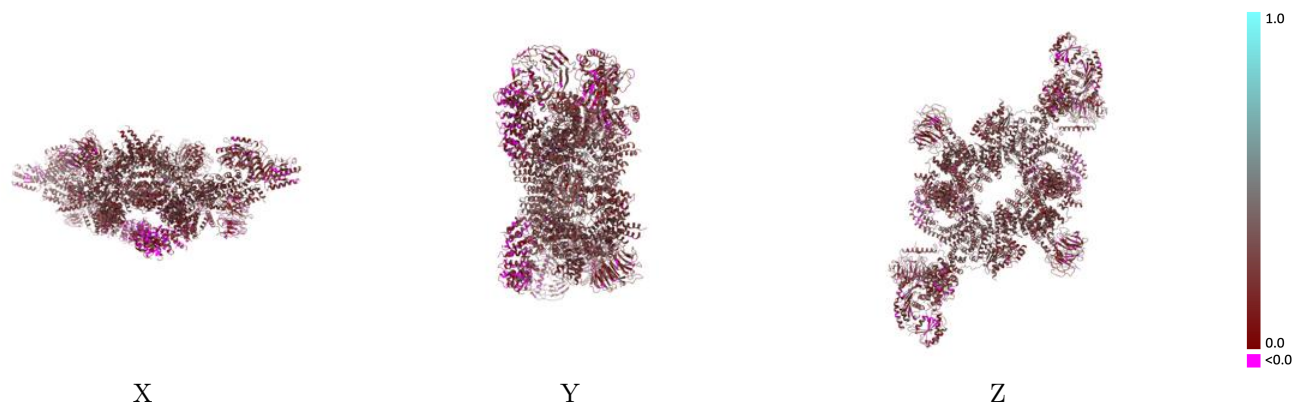
This section contains information regarding the fit between EMDB map EMD-10132 and PDB model 6SB0. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



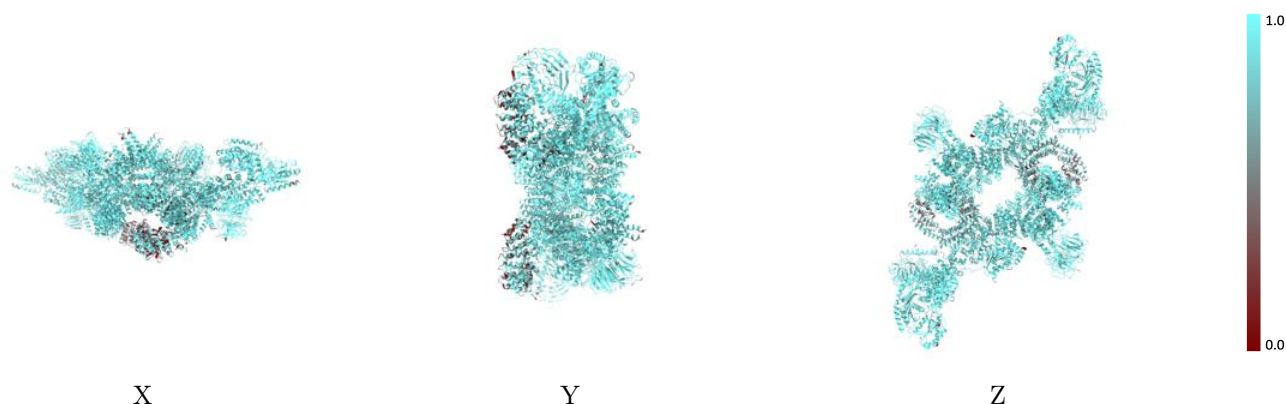
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



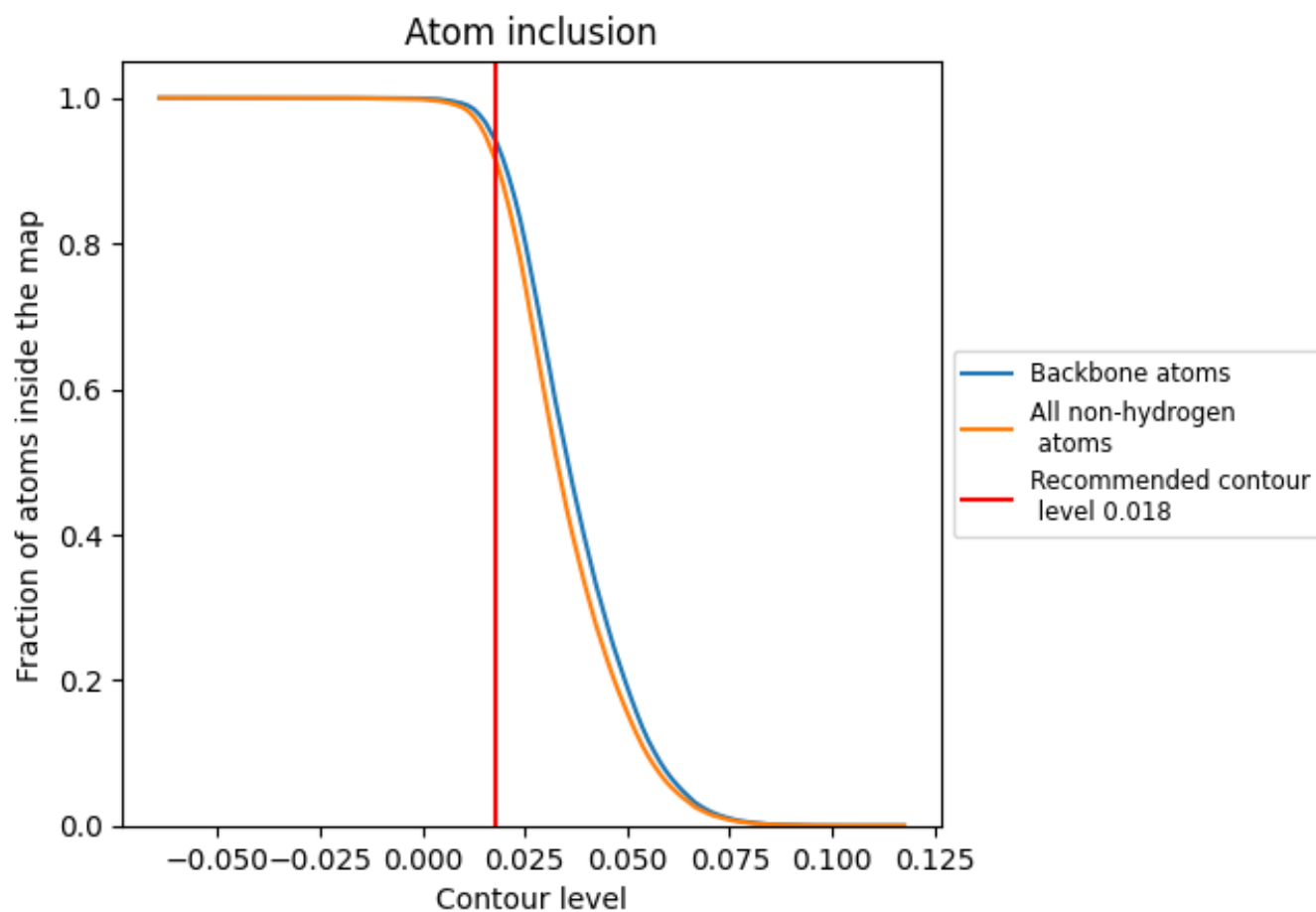
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9128	 0.2370
A	 0.8842	 0.2290
B	 0.8923	 0.2350
C	 0.9333	 0.2270
D	 0.9187	 0.1820
E	 0.9469	 0.2320
H	 0.9494	 0.2240
I	 0.9333	 0.2250
J	 0.9262	 0.1860
N	 0.9499	 0.2640
O	 0.7457	 0.2690
T	 0.7688	 0.2640
Y	 0.9498	 0.2650

