Full wwPDB EM Validation Report (i)

Oct 1, 2024 – 12:18 AM JST

PDB ID	:	5H64
EMDB ID	:	EMD-6668
Title	:	Cryo-EM structure of mTORC1
Authors	:	Yang, H.; Wang, J.; Liu, M.; Chen, X.; Huang, M.; Tan, D.; Dong, M.; Wong, C.C.L.; Wang, J.; Xu, Y.; Wang, H.
Deposited on	:	2016-11-10
Resolution	:	4.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

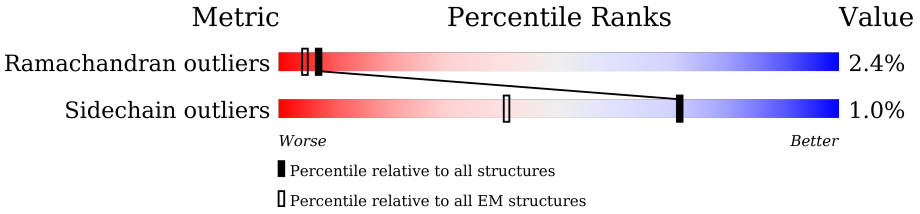
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	13% 77% 5% 18%
1	a	2549	13% 77% 5% 18%
2	B	1335	5% 55% • • 40%
2	b	1335	5% 55% • • 40%
3	C	326	6% 95% • •
3	c	326	7% 95% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 45252 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2101	15617	9886	2788	2849	94	0	0
1	a	2101	15617	9886	2788	2849	94	0	0

- Molecule 2 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	797	4553	2817	832	894	10	0	0
2	b	797	4553	2817	832	894	10	0	0

- Molecule 3 is a protein called Target of rapamycin complex subunit LST8.

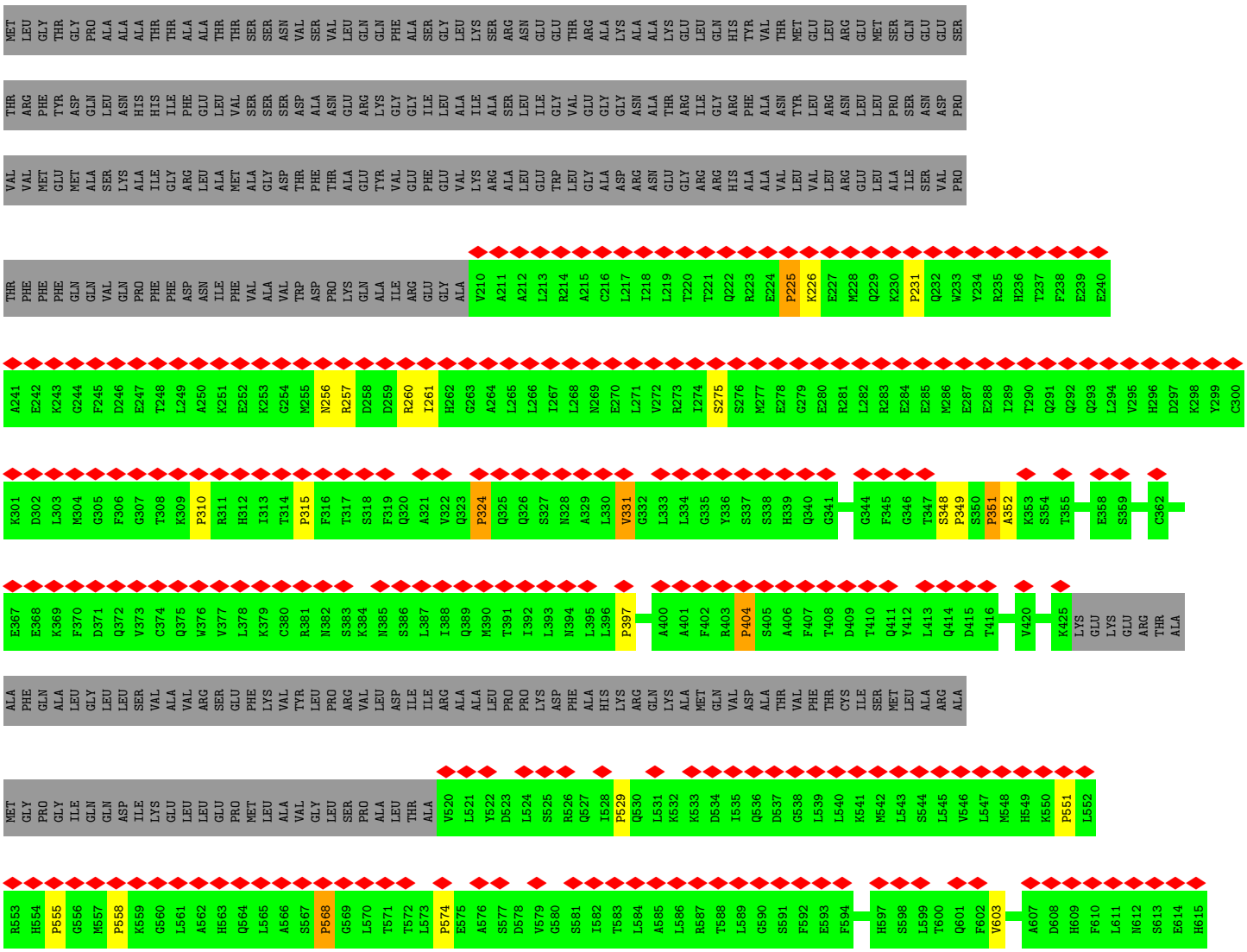
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	317	2456	1526	436	476	18	0	0
3	c	317	2456	1526	436	476	18	0	0

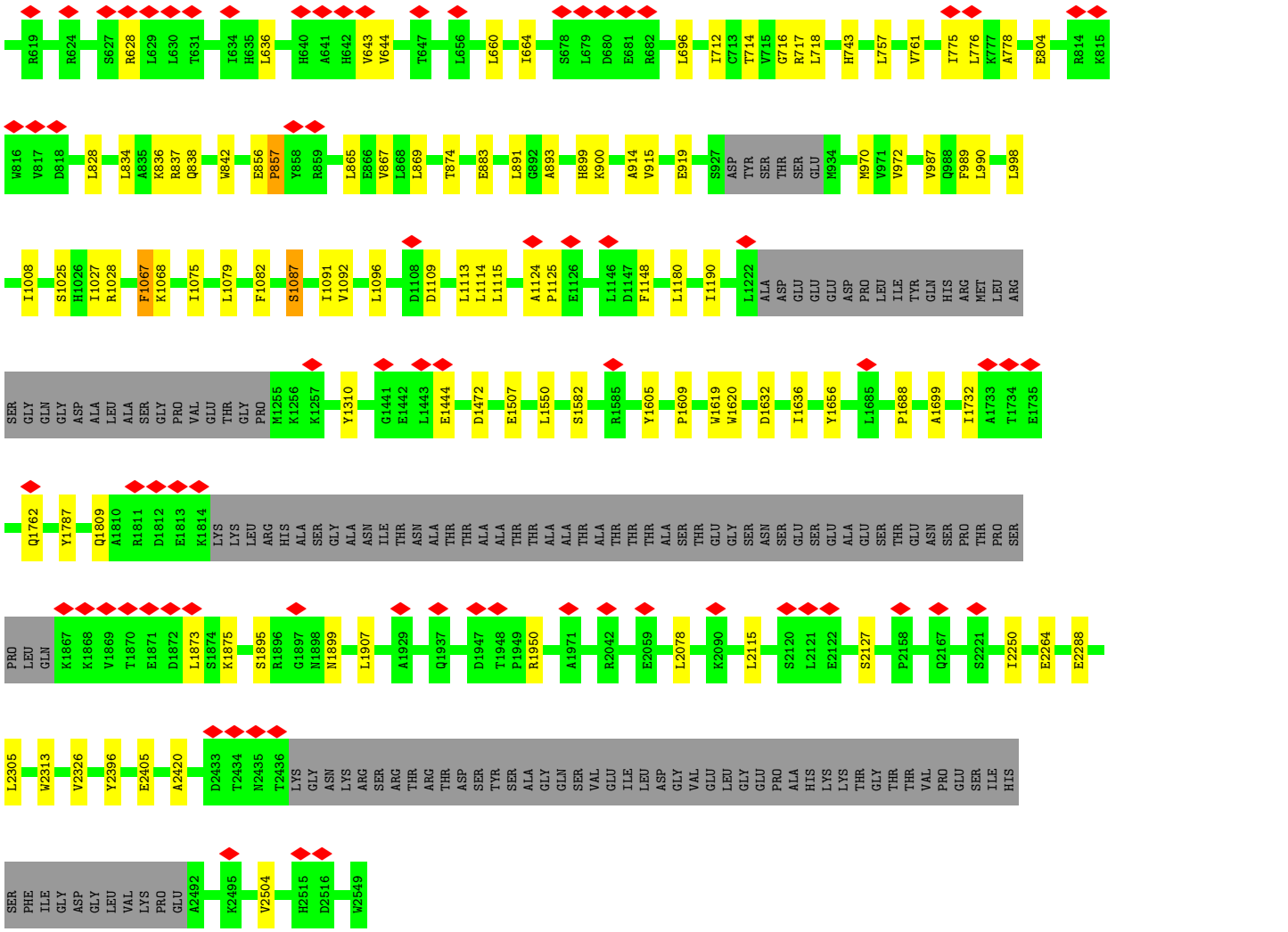
3 Residue-property plots (i)

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

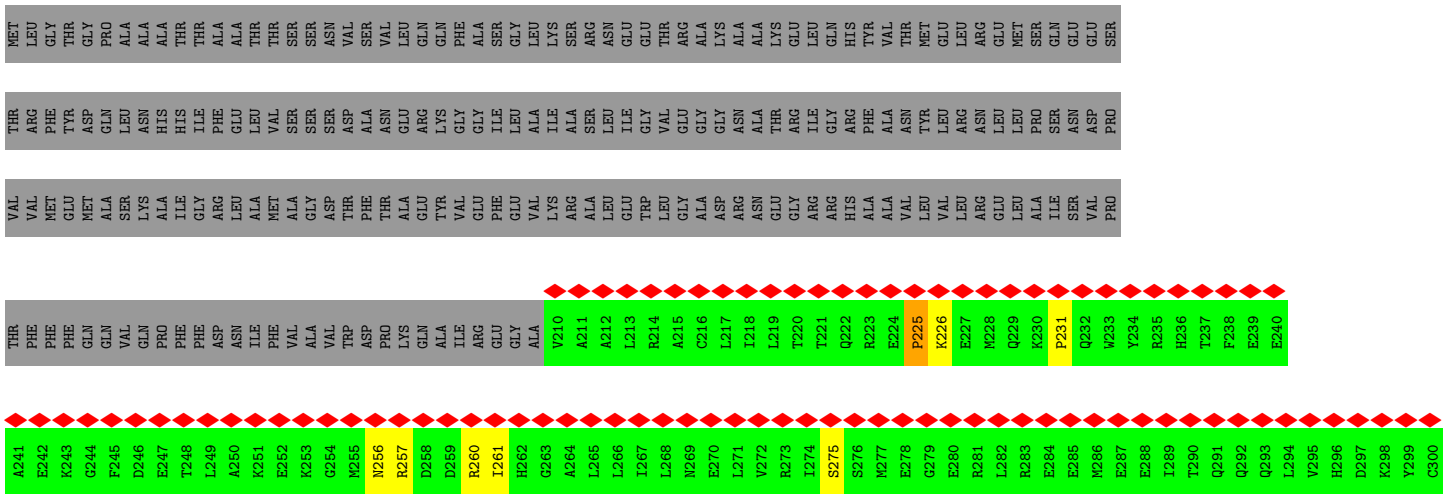
Chain A:

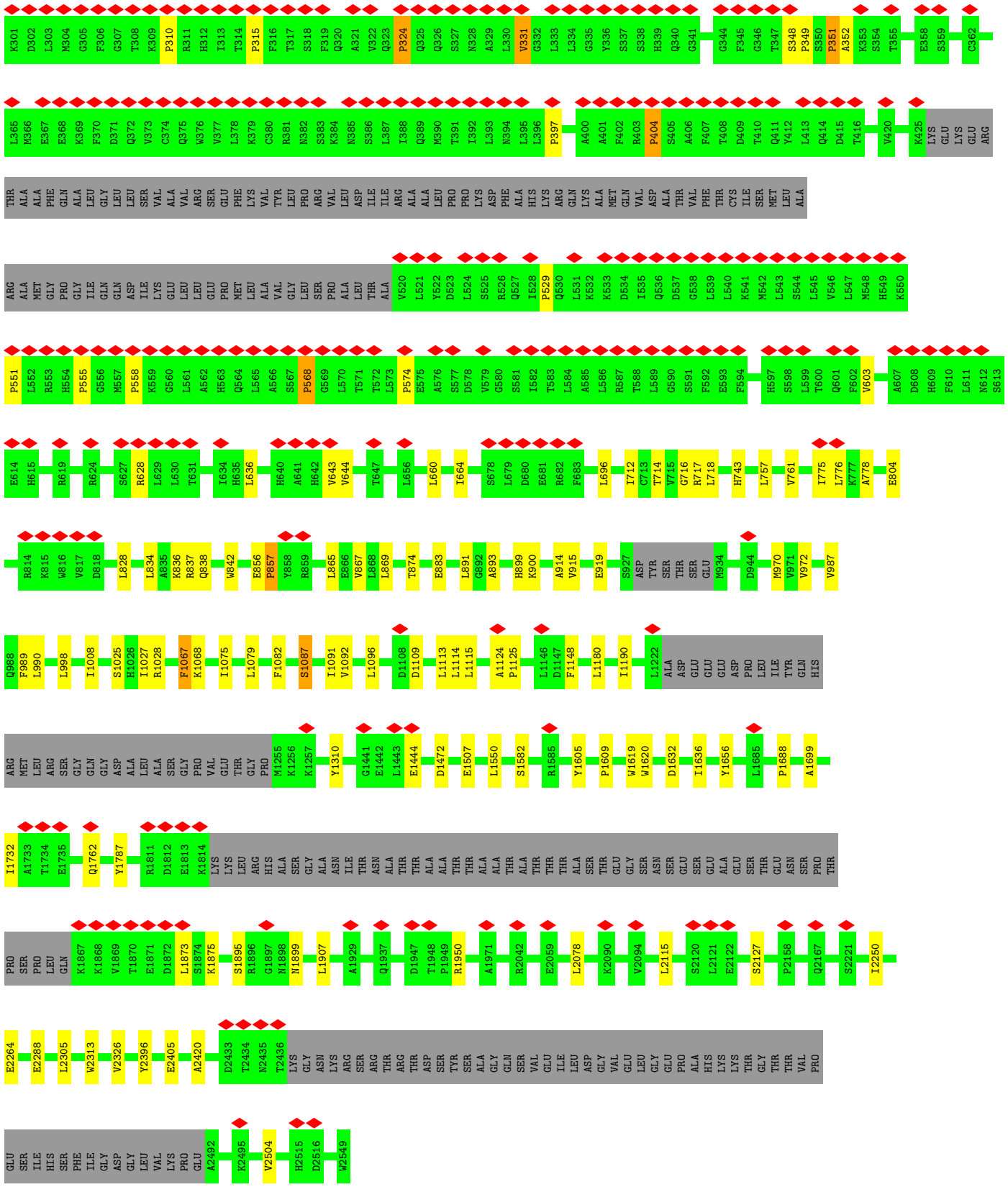




- Molecule 1: Serine/threonine-protein kinase mTOR

Chain a:





- Molecule 2: Regulatory-associated protein of mTOR

Chain B: 5% 55% • • 40%

MET GLU SER GLU MET LEU GLN SER PRO LEU LEU GLY LEU GLY GLU GLU ASP GLU ALA ASP LEU THR ASP TRP ASN LEU PRO LEU ALA PHE MET LYS LYS ARG HIS CYS GLU LYS ILE GLU GLY SER LYS SER LEU ALA GLN SER TRP ARG MET LYS ASP ARG MET LYS THR VAL SER VAL

ALA LEU VAL LEU CYS LEU ASN VAL GLY VAL ASP PRO PRO ASP VAL VAL LYS T78 P90 L91 S92 P95 Q96 Q114 P115 V127 V130 L133 A141 K142 E143 G154 V155 P156 R157 P158 T159 V160 N161 V164 N168 K169 ASN TYR THR GLN TYR ILE PRO LEU

SER ILE TYR ASP LEU GLN THR TRP M186 E216 L217 E218 V219 A220 A221 ILE ASN PRO ASN HIS PRO LEU ALA GLN MET PRO LEU PRO PRO SER MET LYS ASN CYS ILE GLN LEU ALA ALA CYS GLU ALA THR GLU LEU LEU PRO MET ILE P256 D257 D261 L267 THR THR PRO ILE

LYS ILE ALA LEU ARG TRP PHE CYS MET GLN LYS CYS VAL SER LEU VAL PRO GLY VAL THR LEU ASP LEU ILE GLU LYS ILE PRO GLY ARG LEU ASN ASP ARG ARG THR PRO LEU GLY GLU LEU ASN TRP ILE PHE THR ALA ILE THR ASP THR ILE ALA TRP ASN VAL LEU PRO ARG ASP

LEU PHE GLN LYS LEU PHE ARG GLN D340 V343 L352 P371 A402 F408 L420 T421 E425 P429 P430 Q438 VAL LEU L441 V444 H445 I472 F473 P474 R488 P489 F493 I494 M495 A496 K497 I498 V510 V541 T548 GLY GLN GLU ALA CYS

LEU GLN GLY ASN LEU ILE ALA ILE CYS LEU GLU GLN LEU ASN ASP PRO HIS PRO LEU LEU ARG GLN TRP VAL ALA ILE CYS LEU GLY ARG I584 S630 V644 R727 A728 E747 N758 LEU SER THR SER SER SER ALA SER SER THR LEU GLY SER PRO GLU ASN GLU GLU

HIS I778 I784 M787 R788 S795 L796 V807 I811 V814 LEU LEU HIS LEU ALA ALA ASP PRO TYR PRO GLU VAL SER ASP VAL ALA MET LYS VAL LEU ASN SER ILE ALA TYR LYS ALA THR VAL ASN ALA ARG PRO GLN ARG VAL LEU ASP THR SER SER LEU THR GLN

SER ALA PRO ALA SER PRO THR ASN LYS GLY VAL HIS ILE HIS GLN ALA GLY GLY SER P878 P879 P896 V897 P902 S903 G904 ARG PRO GLY THR THR GLY PRO ALA GLY ALA GLN TYR THR P918 F923 P924 R925 D931 LYS GLY PRO GLU GLN THR ALA ASP ASP ALA ASP ASP

ALA ALA GLY HIS LYS S949 F950 A953 T954 V955 Q956 T957 GLY PHE CYS ASP TRP SER ALA ARG TYR PHE ALA GLN PRO VAL MET LYS ILE PRO GLU GLU HIS ASP LEU GLU SER GLN ILE ARG LYS GLU ARG GLU TRP ARG PHE LEU ARG ASN SER ARG VAL ARG ARG GLN ALA GLN GLN

VAL ILE GLN LYS GLY ILE THR ARG LEU ASP ASP GLN ILE PHE LEU ASN ARG ASN PRO GLY VAL PRO SER VAL VAL LYS PHE HIS PRO F1034 T1035 P1036 A1039 V1040 D1050 W1051 E1052 K1053 L1057 H1061 ASN GLY ASN P1065 R1066 Y1067 T1068 R1069 V1070 Y1075 L1076 N1077 GLY GLN ASP

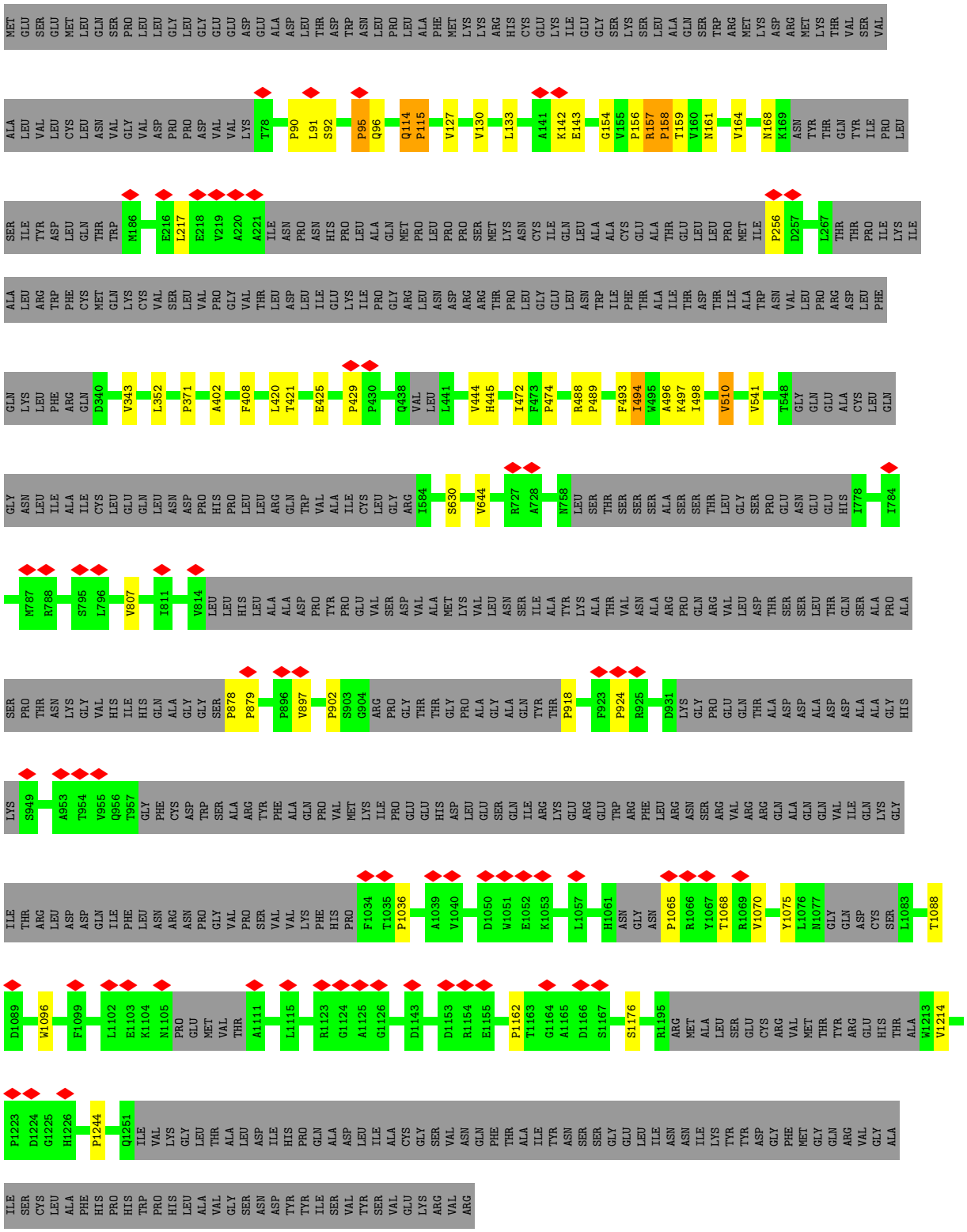
CYS SER L1083 T1088 D1089 W1096 F1099 L1102 E1103 K1104 N1105 PRO GLU MET VAL THR A1111 T1122 R1123 G1124 A1125 G1126 D1143 D1153 R1154 E1155 P1162 T1163 G1164 A1165 D1166 S1167 S1176 R1195 ARG MET ALA LEU SER GLU CYS ARG VAL MET THR TYR ARG GLU HIS THR

ALA W1213 V1214 P1223 D1224 G1225 H1226 P1244 Q1251 ILE VAL LYS GLY LEU THR ALA LEU ASP ILE HIS PRO GLN ALA ASP LEU ILE ALA CYS GLY SER VAL ASN GLN PHE THR ALA ILE TYR ASN SER SER GLY GLU LEU ILE ASN ASN ILE LYS TYR TYR ASP GLY PHE MET GLY GLN

ARG VAL GLY ALA ILE SER CYS LEU ALA PHE HIS PRO HIS TRP PRO HIS LEU ALA VAL GLY SER ASN ASP TYR TYR ILE SER VAL TYR SER VAL GLU LYS ARG VAL ARG

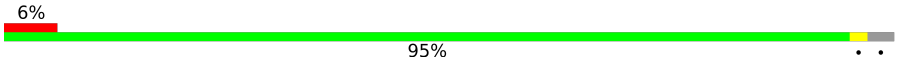
• Molecule 2: Regulatory-associated protein of mTOR

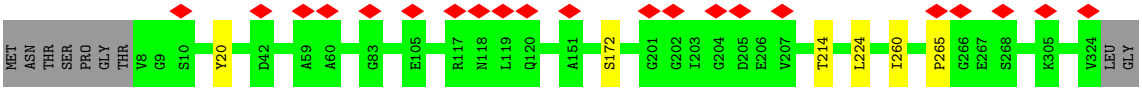
Chain b: 5% 55% • • 40%



• Molecule 3: Target of rapamycin complex subunit LST8

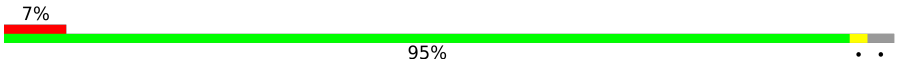
Chain C:

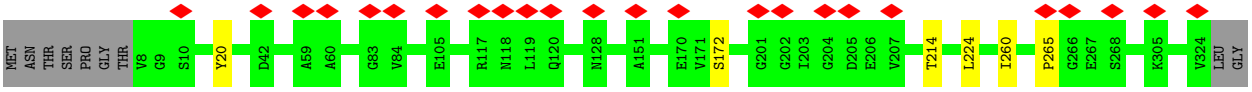




• Molecule 3: Target of rapamycin complex subunit LST8

Chain c:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	115039	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 ($e^-/Å^2$)	8.25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0142	Depositor
Map size (Å)	391.962, 391.962, 391.962	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.56	4/15910 (0.0%)	0.78	38/21634 (0.2%)
1	a	0.56	4/15910 (0.0%)	0.78	38/21634 (0.2%)
2	B	0.40	1/4567 (0.0%)	0.73	13/6217 (0.2%)
2	b	0.40	1/4567 (0.0%)	0.73	13/6217 (0.2%)
3	C	0.49	0/2514	0.68	1/3426 (0.0%)
3	c	0.49	0/2514	0.68	1/3426 (0.0%)
All	All	0.53	10/45982 (0.0%)	0.76	104/62554 (0.2%)

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	47
1	a	0	46
2	B	0	14
2	b	0	14
3	C	0	4
3	c	0	4
All	All	0	129

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2313	TRP	CB-CG	-7.38	1.36	1.50
1	a	2313	TRP	CB-CG	-7.37	1.36	1.50
1	A	1619	TRP	CB-CG	-6.24	1.39	1.50
1	a	1619	TRP	CB-CG	-6.22	1.39	1.50
1	a	842	TRP	CB-CG	-5.75	1.40	1.50
1	A	842	TRP	CB-CG	-5.71	1.40	1.50
1	a	1620	TRP	CB-CG	-5.34	1.40	1.50
1	A	1620	TRP	CB-CG	-5.32	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	115	PRO	N-CD	5.13	1.55	1.47
2	B	115	PRO	N-CD	5.12	1.55	1.47

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	114	GLN	C-N-CD	-17.81	81.41	120.60
2	B	114	GLN	C-N-CD	-17.81	81.41	120.60
1	a	1113	LEU	CA-CB-CG	-10.98	90.05	115.30
1	A	1113	LEU	CA-CB-CG	-10.97	90.06	115.30
2	b	115	PRO	CA-N-CD	-10.09	97.38	111.50
2	B	115	PRO	CA-N-CD	-10.08	97.39	111.50
2	B	158	PRO	CA-N-CD	-9.13	98.72	111.50
2	b	158	PRO	CA-N-CD	-9.12	98.73	111.50
1	A	757	LEU	CA-CB-CG	-7.50	98.06	115.30
1	a	757	LEU	CA-CB-CG	-7.49	98.06	115.30
2	b	217	LEU	CB-CG-CD1	-7.10	98.93	111.00
2	B	217	LEU	CB-CG-CD1	-7.08	98.96	111.00
1	a	225	PRO	N-CA-CB	6.82	111.48	103.30
1	A	225	PRO	N-CA-CB	6.81	111.48	103.30
1	A	915	VAL	C-N-CA	6.64	138.29	121.70
1	a	915	VAL	C-N-CA	6.63	138.28	121.70
1	A	1114	LEU	CA-CB-CG	-6.61	100.09	115.30
1	a	1114	LEU	CA-CB-CG	-6.61	100.10	115.30
1	A	555	PRO	N-CA-CB	6.58	111.19	103.30
1	a	2115	LEU	CB-CG-CD1	-6.54	99.88	111.00
1	A	2115	LEU	CB-CG-CD1	-6.54	99.88	111.00
1	a	555	PRO	N-CA-CB	6.53	111.13	103.30
2	B	156	PRO	N-CA-CB	6.53	111.13	103.30
2	b	156	PRO	N-CA-CB	6.53	111.13	103.30
2	b	157	ARG	C-N-CD	-6.41	106.50	120.60
2	B	157	ARG	C-N-CD	-6.41	106.51	120.60
2	B	352	LEU	C-N-CA	6.34	137.54	121.70
2	b	352	LEU	C-N-CA	6.33	137.54	121.70
2	B	878	PRO	N-CA-CB	6.33	110.89	103.30
2	b	878	PRO	N-CA-CB	6.33	110.89	103.30
1	A	891	LEU	CA-CB-CG	-6.29	100.83	115.30
1	a	891	LEU	CA-CB-CG	-6.29	100.83	115.30
1	a	529	PRO	N-CA-CB	6.27	110.83	103.30
1	a	2305	LEU	CA-CB-CG	-6.25	100.92	115.30
1	A	529	PRO	N-CA-CB	6.25	110.80	103.30
1	A	2305	LEU	CA-CB-CG	-6.23	100.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	256	PRO	N-CA-CB	6.22	110.77	103.30
1	a	1180	LEU	CA-CB-CG	-6.22	100.99	115.30
1	A	1180	LEU	CA-CB-CG	-6.22	101.00	115.30
2	B	256	PRO	N-CA-CB	6.16	110.69	103.30
1	A	1873	LEU	CA-CB-CG	6.11	129.35	115.30
2	B	420	LEU	CA-CB-CG	-6.11	101.25	115.30
2	b	420	LEU	CA-CB-CG	-6.11	101.25	115.30
1	a	1873	LEU	CA-CB-CG	6.10	129.33	115.30
1	A	869	LEU	CA-CB-CG	6.09	129.30	115.30
1	a	869	LEU	CA-CB-CG	6.06	129.25	115.30
1	A	310	PRO	N-CA-CB	6.03	110.54	103.30
1	A	551	PRO	N-CA-CB	6.03	110.54	103.30
1	a	310	PRO	N-CA-CB	6.03	110.54	103.30
1	A	225	PRO	C-N-CA	6.01	136.74	121.70
1	a	551	PRO	N-CA-CB	6.01	110.52	103.30
1	a	225	PRO	C-N-CA	6.00	136.71	121.70
1	a	696	LEU	CA-CB-CG	-5.99	101.53	115.30
1	A	351	PRO	N-CA-CB	5.98	110.48	103.30
1	A	696	LEU	CA-CB-CG	-5.97	101.56	115.30
1	a	351	PRO	N-CA-CB	5.97	110.47	103.30
1	A	558	PRO	N-CA-CB	5.95	110.44	103.30
1	A	998	LEU	CA-CB-CG	-5.93	101.66	115.30
1	a	998	LEU	CA-CB-CG	-5.92	101.68	115.30
1	a	558	PRO	N-CA-CB	5.91	110.39	103.30
2	b	133	LEU	CA-CB-CG	-5.84	101.87	115.30
1	A	397	PRO	N-CA-CB	5.83	110.30	103.30
2	B	133	LEU	CA-CB-CG	-5.83	101.89	115.30
1	a	397	PRO	N-CA-CB	5.82	110.29	103.30
1	a	1609	PRO	N-CA-CB	5.82	110.29	103.30
1	a	1688	PRO	C-N-CA	-5.81	107.19	121.70
1	A	1609	PRO	N-CA-CB	5.80	110.27	103.30
1	A	1688	PRO	C-N-CA	-5.80	107.19	121.70
1	a	404	PRO	N-CA-CB	5.78	110.23	103.30
1	A	404	PRO	N-CA-CB	5.77	110.23	103.30
1	A	231	PRO	N-CA-CB	5.75	110.20	103.30
1	a	231	PRO	N-CA-CB	5.74	110.19	103.30
1	a	1550	LEU	CA-CB-CG	-5.66	102.28	115.30
1	A	1550	LEU	CA-CB-CG	-5.66	102.29	115.30
2	B	879	PRO	N-CA-CB	5.60	110.02	103.30
1	a	324	PRO	N-CA-CB	5.60	110.02	103.30
1	a	1096	LEU	CA-CB-CG	-5.59	102.43	115.30
2	b	879	PRO	N-CA-CB	5.58	110.00	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1096	LEU	CA-CB-CG	-5.58	102.47	115.30
1	A	324	PRO	N-CA-CB	5.58	109.99	103.30
1	a	315	PRO	N-CA-CB	5.51	109.92	103.30
1	A	315	PRO	N-CA-CB	5.50	109.89	103.30
1	a	574	PRO	N-CA-CB	5.46	109.85	103.30
1	a	1190	ILE	C-N-CA	5.45	135.33	121.70
1	A	574	PRO	N-CA-CB	5.44	109.82	103.30
1	A	1190	ILE	C-N-CA	5.43	135.28	121.70
1	A	349	PRO	N-CA-CB	5.42	109.80	103.30
1	A	1087	SER	C-N-CD	-5.41	108.69	120.60
1	a	349	PRO	N-CA-CB	5.40	109.78	103.30
1	a	1087	SER	C-N-CD	-5.39	108.73	120.60
1	a	1115	LEU	CA-CB-CG	-5.36	102.97	115.30
1	A	1115	LEU	CA-CB-CG	-5.36	102.98	115.30
1	a	828	LEU	CA-CB-CG	-5.15	103.45	115.30
1	A	828	LEU	CA-CB-CG	-5.15	103.46	115.30
1	A	1907	LEU	CA-CB-CG	-5.15	103.46	115.30
1	a	1907	LEU	CA-CB-CG	-5.14	103.48	115.30
3	C	224	LEU	CA-CB-CG	-5.09	103.59	115.30
3	c	224	LEU	CA-CB-CG	-5.09	103.59	115.30
2	B	510	VAL	C-N-CA	5.08	134.41	121.70
2	b	510	VAL	C-N-CA	5.08	134.41	121.70
1	A	636	LEU	CA-CB-CG	-5.08	103.62	115.30
1	a	636	LEU	CA-CB-CG	-5.08	103.62	115.30
1	A	568	PRO	N-CA-CB	5.01	109.31	103.30
1	a	568	PRO	N-CA-CB	5.01	109.31	103.30

There are no chirality outliers.

All (129) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1025	SER	Peptide
1	A	1028	ARG	Peptide
1	A	1067	PHE	Peptide
1	A	1075	ILE	Peptide
1	A	1082	PHE	Peptide
1	A	1087	SER	Peptide
1	A	1109	ASP	Peptide
1	A	1124	ALA	Peptide
1	A	1125	PRO	Peptide
1	A	1148	PHE	Peptide
1	A	1310	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	1444	GLU	Peptide
1	A	1472	ASP	Peptide
1	A	1582	SER	Peptide
1	A	1605	TYR	Peptide
1	A	1732	ILE	Peptide
1	A	1762	GLN	Peptide
1	A	1787	TYR	Peptide
1	A	1809	GLN	Peptide
1	A	1895	SER	Peptide
1	A	1899	ASN	Peptide
1	A	1950	ARG	Peptide
1	A	2127	SER	Peptide
1	A	226	LYS	Peptide
1	A	257	ARG	Peptide
1	A	260	ARG	Peptide
1	A	261	ILE	Peptide
1	A	275	SER	Peptide
1	A	324	PRO	Peptide
1	A	331	VAL	Peptide
1	A	352	ALA	Peptide
1	A	603	VAL	Peptide
1	A	628	ARG	Peptide
1	A	714	THR	Peptide
1	A	716	GLY	Peptide
1	A	718	LEU	Peptide
1	A	776	LEU	Peptide
1	A	836	LYS	Peptide
1	A	856	GLU	Peptide
1	A	857	PRO	Peptide
1	A	874	THR	Peptide
1	A	899	HIS	Peptide
1	A	900	LYS	Peptide
1	A	914	ALA	Peptide
1	A	970	MET	Peptide
1	A	989	PHE	Peptide
1	A	990	LEU	Peptide
2	B	1070	VAL	Peptide
2	B	1096	TRP	Peptide
2	B	114	GLN	Peptide
2	B	157	ARG	Peptide
2	B	161	ASN	Peptide
2	B	343	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	B	371	PRO	Peptide
2	B	408	PHE	Peptide
2	B	429	PRO	Peptide
2	B	445	HIS	Peptide
2	B	474	PRO	Peptide
2	B	494	ILE	Peptide
2	B	498	ILE	Peptide
2	B	644	VAL	Peptide
3	C	172	SER	Peptide
3	C	20	TYR	Peptide
3	C	214	THR	Peptide
3	C	260	ILE	Peptide
1	a	1025	SER	Peptide
1	a	1028	ARG	Peptide
1	a	1067	PHE	Peptide
1	a	1075	ILE	Peptide
1	a	1082	PHE	Peptide
1	a	1087	SER	Peptide
1	a	1109	ASP	Peptide
1	a	1124	ALA	Peptide
1	a	1125	PRO	Peptide
1	a	1148	PHE	Peptide
1	a	1310	TYR	Peptide
1	a	1444	GLU	Peptide
1	a	1472	ASP	Peptide
1	a	1582	SER	Peptide
1	a	1605	TYR	Peptide
1	a	1732	ILE	Peptide
1	a	1762	GLN	Peptide
1	a	1787	TYR	Peptide
1	a	1895	SER	Peptide
1	a	1899	ASN	Peptide
1	a	1950	ARG	Peptide
1	a	2127	SER	Peptide
1	a	226	LYS	Peptide
1	a	257	ARG	Peptide
1	a	260	ARG	Peptide
1	a	261	ILE	Peptide
1	a	275	SER	Peptide
1	a	324	PRO	Peptide
1	a	331	VAL	Peptide
1	a	352	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	a	603	VAL	Peptide
1	a	628	ARG	Peptide
1	a	714	THR	Peptide
1	a	716	GLY	Peptide
1	a	718	LEU	Peptide
1	a	776	LEU	Peptide
1	a	836	LYS	Peptide
1	a	856	GLU	Peptide
1	a	857	PRO	Peptide
1	a	874	THR	Peptide
1	a	899	HIS	Peptide
1	a	900	LYS	Peptide
1	a	914	ALA	Peptide
1	a	970	MET	Peptide
1	a	989	PHE	Peptide
1	a	990	LEU	Peptide
2	b	1070	VAL	Peptide
2	b	1096	TRP	Peptide
2	b	114	GLN	Peptide
2	b	157	ARG	Peptide
2	b	161	ASN	Peptide
2	b	343	VAL	Peptide
2	b	371	PRO	Peptide
2	b	408	PHE	Peptide
2	b	429	PRO	Peptide
2	b	445	HIS	Peptide
2	b	474	PRO	Peptide
2	b	494	ILE	Peptide
2	b	498	ILE	Peptide
2	b	644	VAL	Peptide
3	c	172	SER	Peptide
3	c	20	TYR	Peptide
3	c	214	THR	Peptide
3	c	260	ILE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	2089/2549 (82%)	1654 (79%)	386 (18%)	49 (2%)	5 29
1	a	2089/2549 (82%)	1656 (79%)	384 (18%)	49 (2%)	5 29
2	B	767/1335 (58%)	608 (79%)	132 (17%)	27 (4%)	3 21
2	b	767/1335 (58%)	609 (79%)	131 (17%)	27 (4%)	3 21
3	C	315/326 (97%)	281 (89%)	33 (10%)	1 (0%)	37 72
3	c	315/326 (97%)	281 (89%)	33 (10%)	1 (0%)	37 72
All	All	6342/8420 (75%)	5089 (80%)	1099 (17%)	154 (2%)	7 28

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO
1	A	351	PRO
1	A	404	PRO
1	A	568	PRO
1	A	664	ILE
1	A	837	ARG
1	A	1091	ILE
1	A	1092	VAL
2	B	96	GLN
2	B	115	PRO
2	B	143	GLU
2	B	425	GLU
2	B	488	ARG
2	B	489	PRO
2	B	807	VAL
1	a	225	PRO
1	a	351	PRO
1	a	404	PRO
1	a	568	PRO
1	a	664	ILE

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Mol	Chain	Res	Type
1	a	837	ARG
1	a	1091	ILE
1	a	1092	VAL
2	b	96	GLN
2	b	115	PRO
2	b	143	GLU
2	b	425	GLU
2	b	488	ARG
2	b	489	PRO
2	b	807	VAL
1	A	717	ARG
1	A	778	ALA
1	A	838	GLN
1	A	919	GLU
1	A	987	VAL
1	A	1067	PHE
1	A	1068	LYS
2	B	91	LEU
2	B	95	PRO
2	B	142	LYS
2	B	154	GLY
2	B	444	VAL
2	B	496	ALA
1	a	717	ARG
1	a	778	ALA
1	a	838	GLN
1	a	919	GLU
1	a	987	VAL
1	a	1067	PHE
1	a	1068	LYS
2	b	91	LEU
2	b	95	PRO
2	b	142	LYS
2	b	154	GLY
2	b	444	VAL
2	b	496	ALA
1	A	775	ILE
1	A	883	GLU
2	B	494	ILE
1	a	775	ILE
1	a	883	GLU
2	b	494	ILE

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Mol	Chain	Res	Type
1	A	256	ASN
1	A	643	VAL
1	A	743	HIS
1	A	804	GLU
1	A	893	ALA
1	A	972	VAL
1	A	1079	LEU
1	A	1656	TYR
2	B	158	PRO
2	B	168	ASN
2	B	402	ALA
2	B	472	ILE
2	B	510	VAL
1	a	256	ASN
1	a	643	VAL
1	a	743	HIS
1	a	804	GLU
1	a	893	ALA
1	a	972	VAL
1	a	1079	LEU
1	a	1656	TYR
2	b	158	PRO
2	b	168	ASN
2	b	402	ALA
2	b	472	ILE
2	b	510	VAL
2	b	1075	TYR
1	A	857	PRO
1	A	865	LEU
1	A	867	VAL
1	A	1507	GLU
1	A	2078	LEU
1	A	2288	GLU
1	A	2326	VAL
1	A	2396	TYR
1	A	2420	ALA
2	B	493	PHE
2	B	497	LYS
2	B	630	SER
2	B	1075	TYR
2	B	1176	SER
1	a	857	PRO

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Mol	Chain	Res	Type
1	a	865	LEU
1	a	867	VAL
1	a	1507	GLU
1	a	2078	LEU
1	a	2288	GLU
1	a	2326	VAL
1	a	2396	TYR
1	a	2420	ALA
2	b	493	PHE
2	b	497	LYS
2	b	630	SER
2	b	1176	SER
1	A	834	LEU
1	A	1699	ALA
1	A	1875	LYS
1	A	2264	GLU
1	A	2405	GLU
2	B	541	VAL
1	a	834	LEU
1	a	1699	ALA
1	a	1875	LYS
1	a	2264	GLU
1	a	2405	GLU
2	b	541	VAL
1	A	348	SER
1	A	712	ILE
1	a	348	SER
1	a	712	ILE
1	A	331	VAL
1	A	1027	ILE
1	a	331	VAL
1	a	1027	ILE
1	A	761	VAL
1	A	1008	ILE
1	A	1636	ILE
2	B	130	VAL
2	B	164	VAL
1	a	761	VAL
1	a	1008	ILE
1	a	1636	ILE
2	b	130	VAL
2	b	164	VAL

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Mol	Chain	Res	Type
1	A	644	VAL
1	A	2250	ILE
1	A	2504	VAL
3	C	265	PRO
1	a	644	VAL
1	a	2250	ILE
1	a	2504	VAL
3	c	265	PRO

5.3.2 Protein sidechains (i)

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	1487/2220 (67%)	1485 (100%)	2 (0%)	92 95
1	a	1487/2220 (67%)	1485 (100%)	2 (0%)	92 95
2	B	185/1163 (16%)	167 (90%)	18 (10%)	6 22
2	b	177/1163 (15%)	160 (90%)	17 (10%)	7 22
3	C	269/276 (98%)	269 (100%)	0	100 100
3	c	269/276 (98%)	269 (100%)	0	100 100
All	All	3874/7318 (53%)	3835 (99%)	39 (1%)	71 81

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	660	LEU
1	A	1632	ASP
2	B	90	PRO
2	B	92	SER
2	B	95	PRO
2	B	127	VAL
2	B	159	THR
2	B	421	THR
2	B	897	VAL
2	B	902	PRO

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Mol	Chain	Res	Type
2	B	918	PRO
2	B	924	PRO
2	B	1036	PRO
2	B	1040	VAL
2	B	1065	PRO
2	B	1068	THR
2	B	1088	THR
2	B	1162	PRO
2	B	1214	VAL
2	B	1244	PRO
1	a	660	LEU
1	a	1632	ASP
2	b	90	PRO
2	b	92	SER
2	b	95	PRO
2	b	127	VAL
2	b	159	THR
2	b	421	THR
2	b	897	VAL
2	b	902	PRO
2	b	918	PRO
2	b	924	PRO
2	b	1036	PRO
2	b	1065	PRO
2	b	1068	THR
2	b	1088	THR
2	b	1162	PRO
2	b	1214	VAL
2	b	1244	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	HIS
1	A	601	GLN
1	A	609	HIS
1	A	612	ASN
1	A	686	HIS
1	A	694	GLN
1	A	701	ASN
1	A	722	ASN
1	A	743	HIS

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Mol	Chain	Res	Type
1	A	829	GLN
1	A	966	HIS
1	A	1084	HIS
1	A	1112	HIS
1	A	1196	ASN
1	A	1202	HIS
1	A	1206	HIS
1	A	1405	GLN
1	A	1420	ASN
1	A	1424	GLN
1	A	1439	HIS
1	A	1604	GLN
1	A	1716	HIS
1	A	1718	GLN
1	A	1729	GLN
1	A	1970	GLN
1	A	1988	HIS
1	A	1989	ASN
1	A	1992	ASN
1	A	1997	ASN
1	A	2055	HIS
1	A	2071	ASN
1	A	2106	HIS
1	A	2147	ASN
1	A	2180	HIS
1	A	2219	ASN
1	A	2265	HIS
1	A	2395	ASN
1	A	2410	HIS
1	A	2428	ASN
1	A	2494	ASN
1	A	2535	HIS
2	B	1105	ASN
2	B	1177	HIS
3	C	132	ASN
3	C	140	GLN
3	C	153	HIS
3	C	164	GLN
3	C	219	HIS
3	C	242	GLN
3	C	251	ASN
1	a	597	HIS

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Mol	Chain	Res	Type
1	a	601	GLN
1	a	609	HIS
1	a	612	ASN
1	a	686	HIS
1	a	694	GLN
1	a	701	ASN
1	a	722	ASN
1	a	743	HIS
1	a	829	GLN
1	a	966	HIS
1	a	1084	HIS
1	a	1112	HIS
1	a	1196	ASN
1	a	1202	HIS
1	a	1206	HIS
1	a	1405	GLN
1	a	1420	ASN
1	a	1424	GLN
1	a	1439	HIS
1	a	1541	HIS
1	a	1604	GLN
1	a	1716	HIS
1	a	1718	GLN
1	a	1729	GLN
1	a	1970	GLN
1	a	1988	HIS
1	a	1989	ASN
1	a	1992	ASN
1	a	1997	ASN
1	a	2055	HIS
1	a	2106	HIS
1	a	2147	ASN
1	a	2180	HIS
1	a	2219	ASN
1	a	2265	HIS
1	a	2395	ASN
1	a	2410	HIS
1	a	2428	ASN
1	a	2494	ASN
1	a	2535	HIS
2	b	1105	ASN
2	b	1177	HIS

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Mol	Chain	Res	Type
3	c	132	ASN
3	c	140	GLN
3	c	153	HIS
3	c	164	GLN
3	c	219	HIS
3	c	242	GLN
3	c	251	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

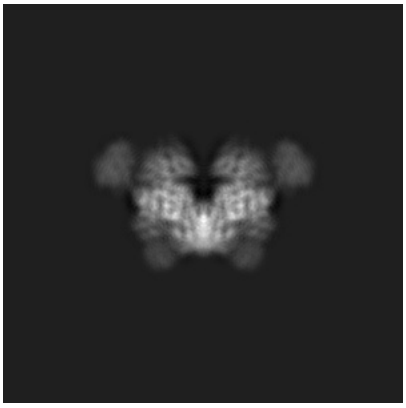
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6668. These allow visual inspection of the internal detail of the map and identification of artifacts.

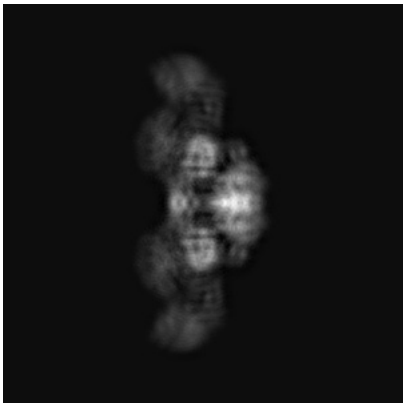
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

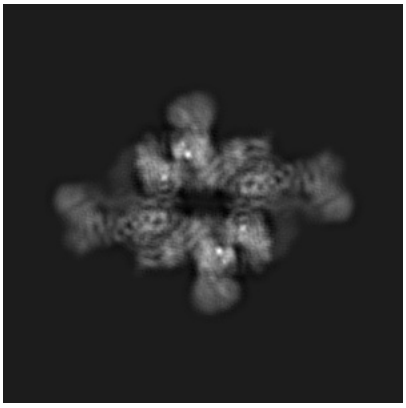
6.1.1 Primary map



X



Y

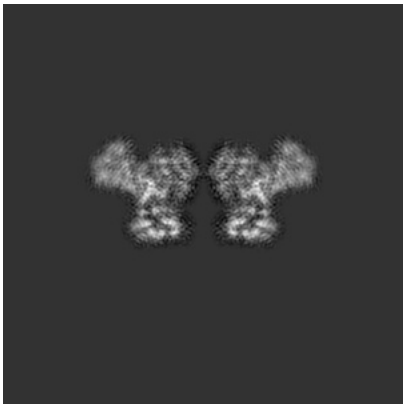


Z

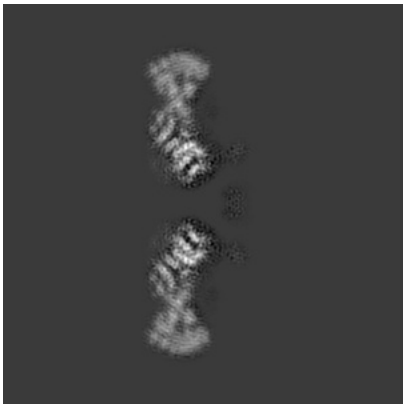
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

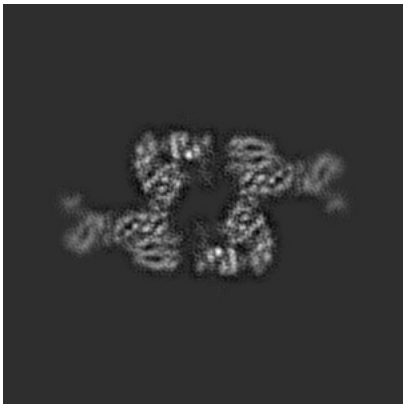
6.2.1 Primary map



X Index: 150



Y Index: 150

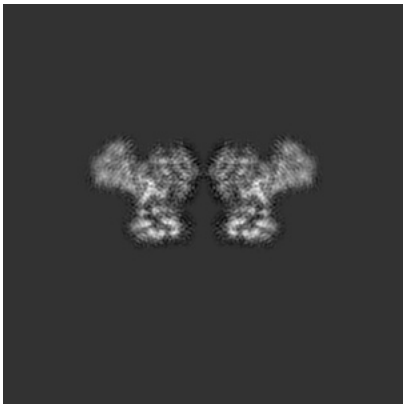


Z Index: 150

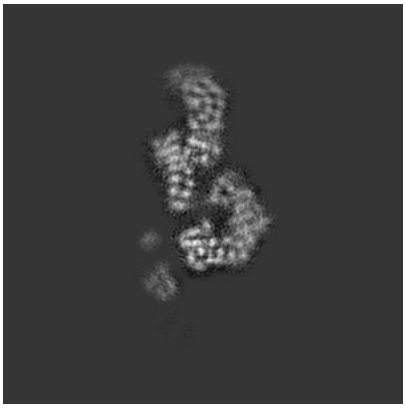
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

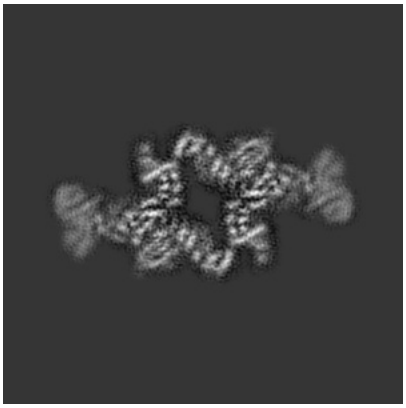
6.3.1 Primary map



X Index: 150



Y Index: 170

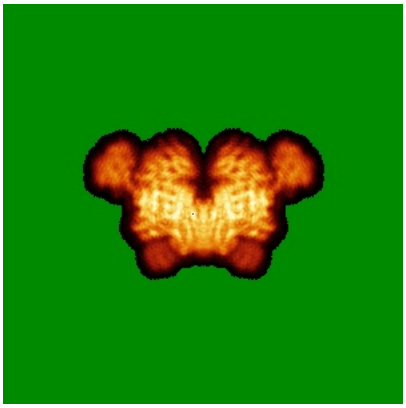


Z Index: 141

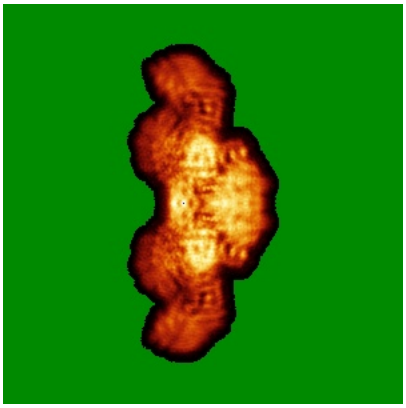
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

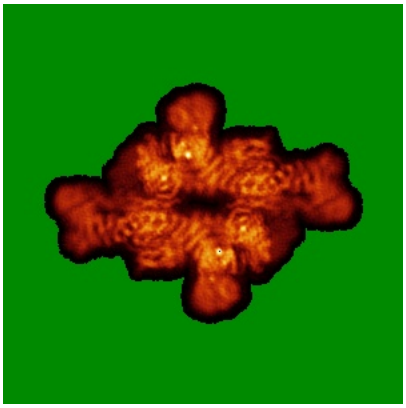
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0142. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

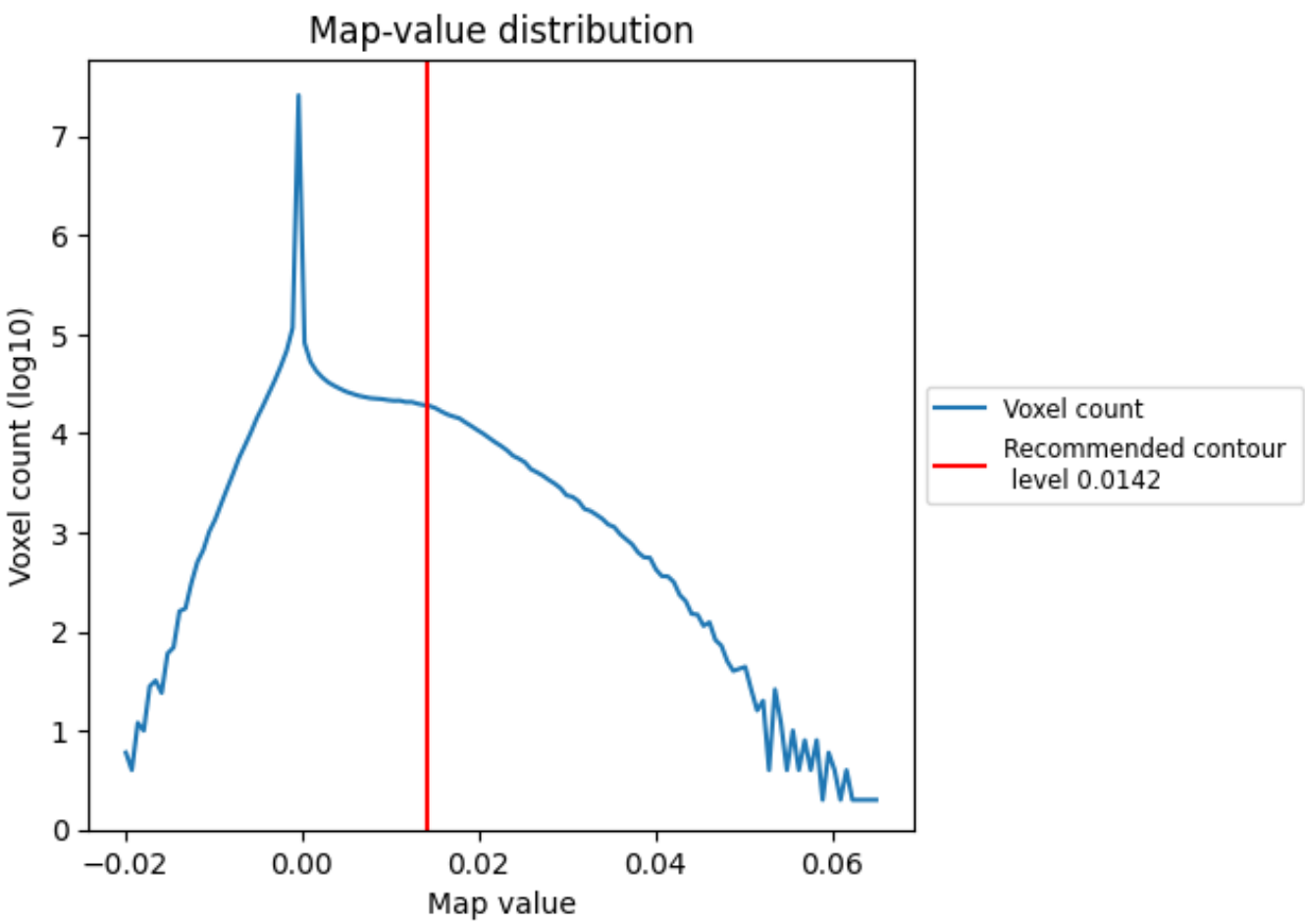
6.6 Mask visualisation (i)

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

7 Map analysis (i)

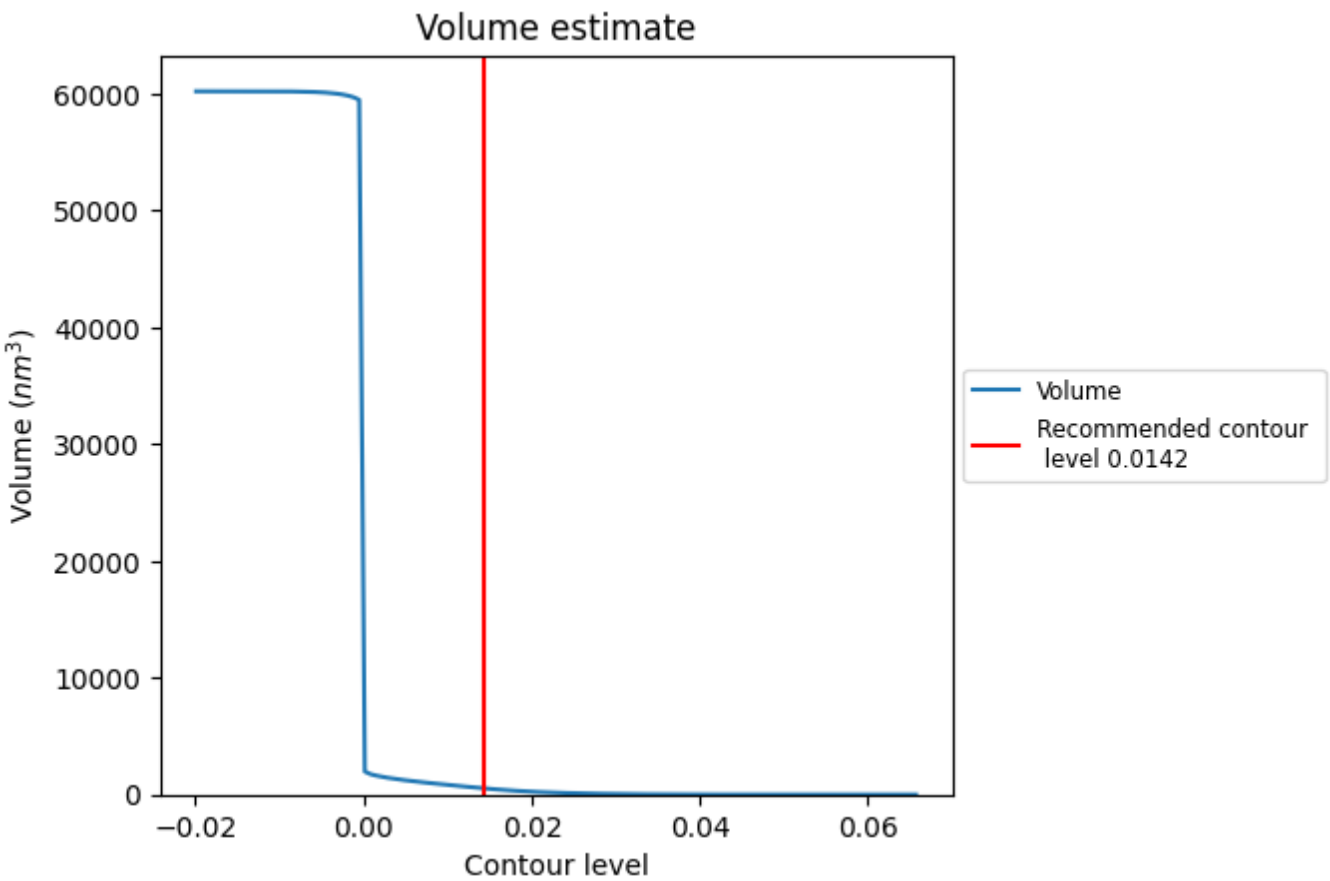
This section contains the results of statistical analysis of the map.

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.

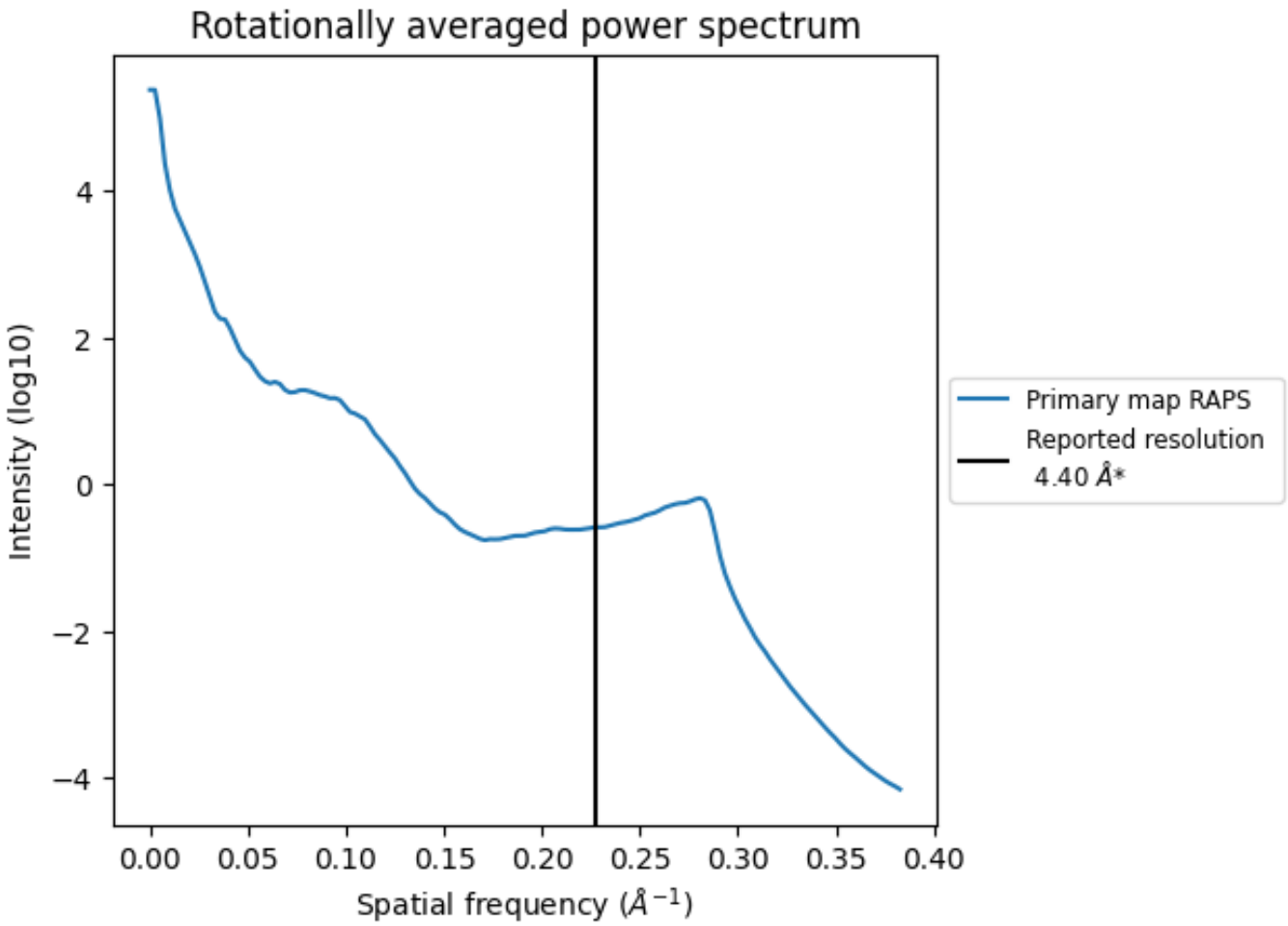
7.2 Volume estimate (i)



The volume at the recommended contour level is 541 nm^3; this corresponds to an approximate mass of 489 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 0.227 Å^{-1}

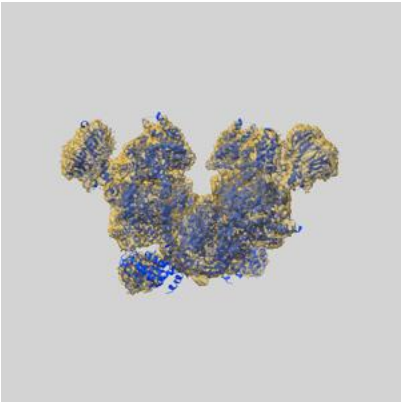
8 Fourier-Shell correlation (i)

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

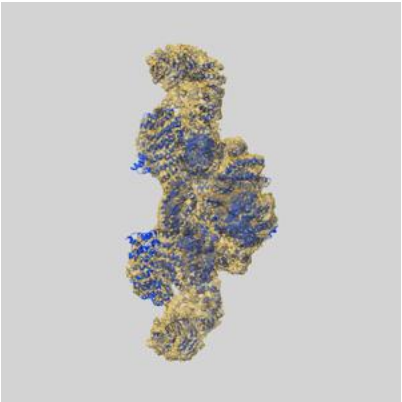
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6668 and PDB model 5H64. Per-residue inclusion information can be found in section 3 on page 4.

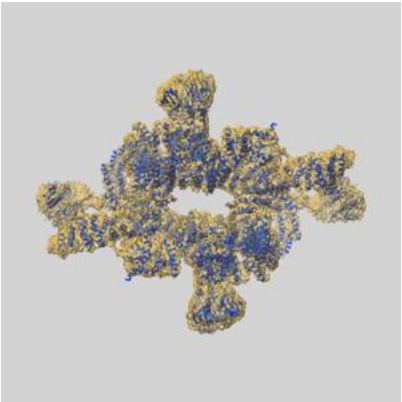
9.1 Map-model overlay (i)



X



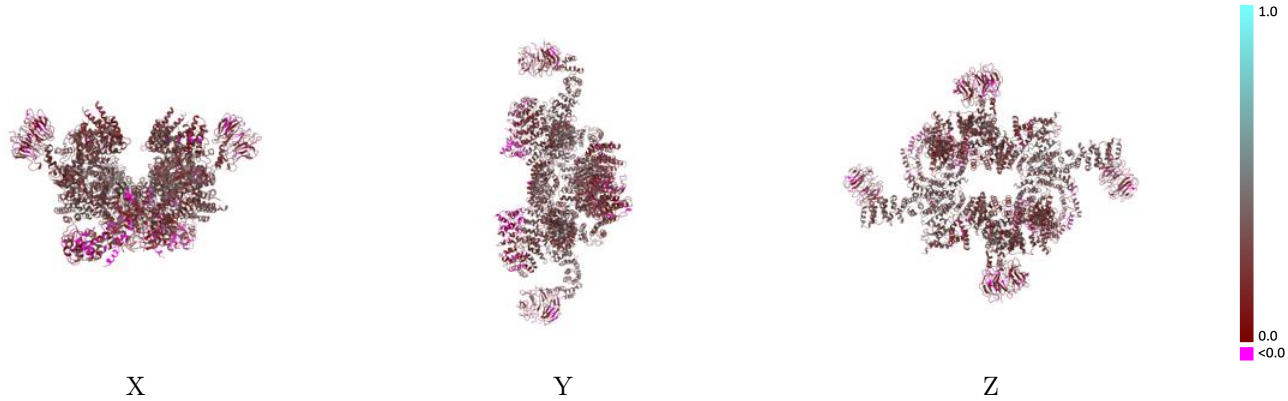
Y



Z

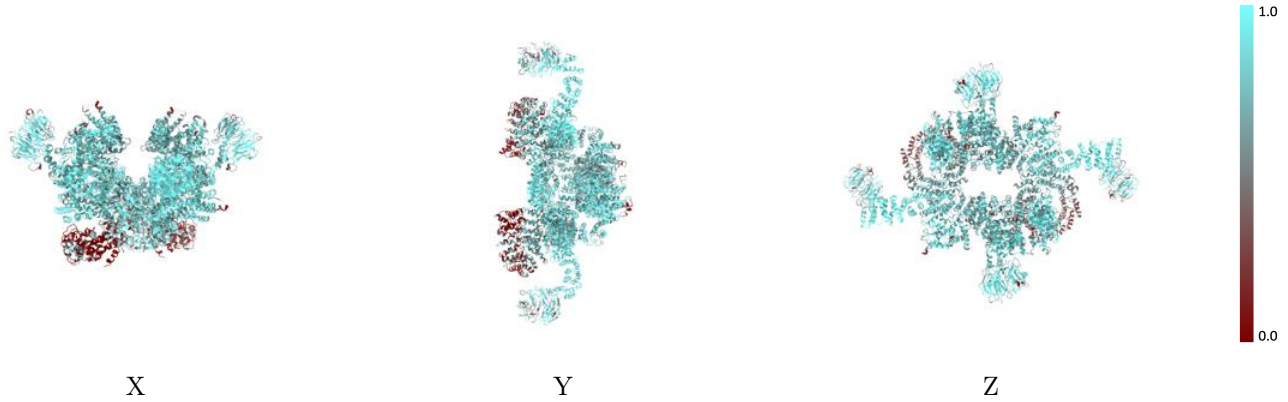
The images above show the 3D surface view of the map at the recommended contour level 0.0142 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



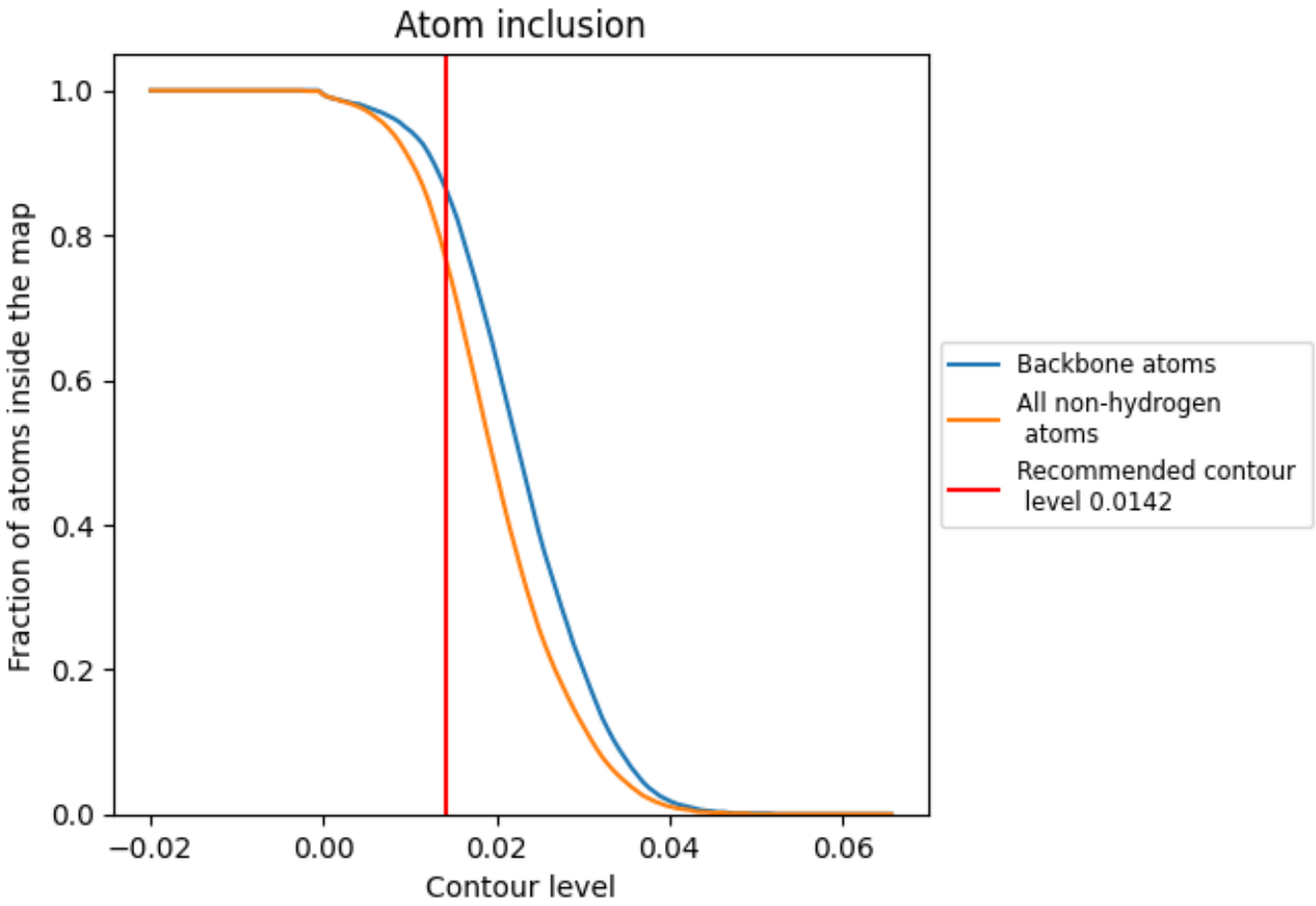
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0142).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0142) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.2490
A	0.7330	0.2560
B	0.8370	0.2700
C	0.8400	0.1710
a	0.7330	0.2550
b	0.8360	0.2700
c	0.8370	0.1680