



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:05 PM UTC

PDB ID : 2X31 / pdb_00002x31
EMDB ID : EMD-1676
Title : Modelling of the complex between subunits BchI and BchD of magnesium chelatase based on single-particle cryo-EM reconstruction at 7.5 ang
Authors : Lunqvist, J.; Elmlund, H.; Peterson Wulff, R.; Berglund, L.; Elmlund, D.; Emanuelsson, C.; Hebert, H.; Willows, R.D.; Hansson, M.; Lindahl, M.; Al-Karadaghi, S.
Deposited on : 2010-01-19
Resolution : 7.50 Å(reported)
Based on initial model : 1G8P

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

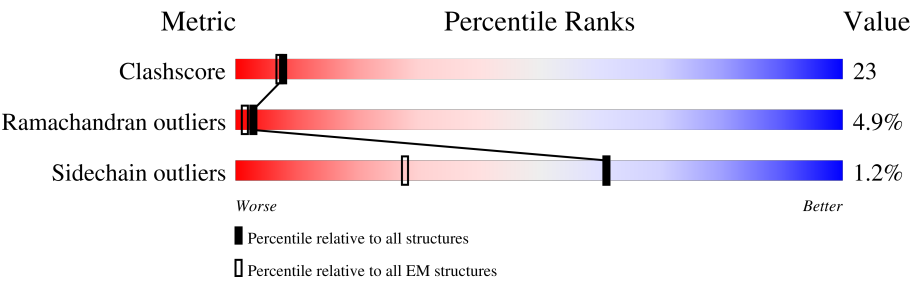
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.50 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	189	99% 59% 38% ..
1	B	189	99% 59% 38% ..
1	C	189	99% 60% 37% ..
1	D	189	99% 58% 39% ..
1	E	189	99% 59% 37% ..
1	F	189	99% 56% 41% ..
2	G	350	92% 57% 33% . 8%
2	H	350	92% 62% 27% . 8%

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Mol	Chain	Length	Quality of chain
2	I	350	92% 57% 34% 8%
2	J	350	92% 62% 27% 8%
2	K	350	92% 57% 34% 8%
2	L	350	92% 62% 27% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22890 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 MAGNESIUM-CHELATASE 60 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	188	Total	C	N	O	S	0	1
			1357	837	255	256	9		
1	B	188	Total	C	N	O	S	0	1
			1357	837	255	256	9		
1	C	188	Total	C	N	O	S	0	1
			1357	837	255	256	9		
1	D	188	Total	C	N	O	S	0	1
			1357	837	255	256	9		
1	E	188	Total	C	N	O	S	0	1
			1357	837	255	256	9		
1	F	188	Total	C	N	O	S	0	1
			1357	837	255	256	9		

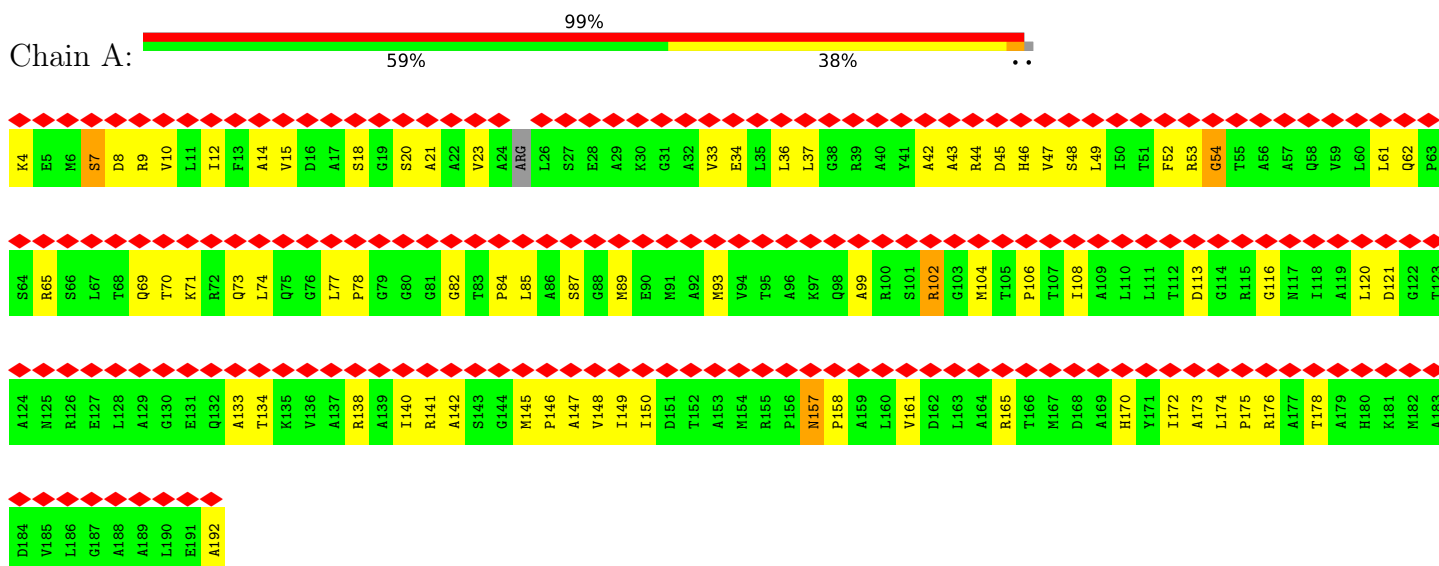
- Molecule 2 is a protein called MAGNESIUM-CHELATASE 38 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	322	Total	C	N	O	S	0	1
			2458	1540	443	467	8		
2	H	322	Total	C	N	O	S	0	1
			2458	1540	443	467	8		
2	I	322	Total	C	N	O	S	0	1
			2458	1540	443	467	8		
2	J	322	Total	C	N	O	S	0	1
			2458	1540	443	467	8		
2	K	322	Total	C	N	O	S	0	1
			2458	1540	443	467	8		
2	L	322	Total	C	N	O	S	0	1
			2458	1540	443	467	8		

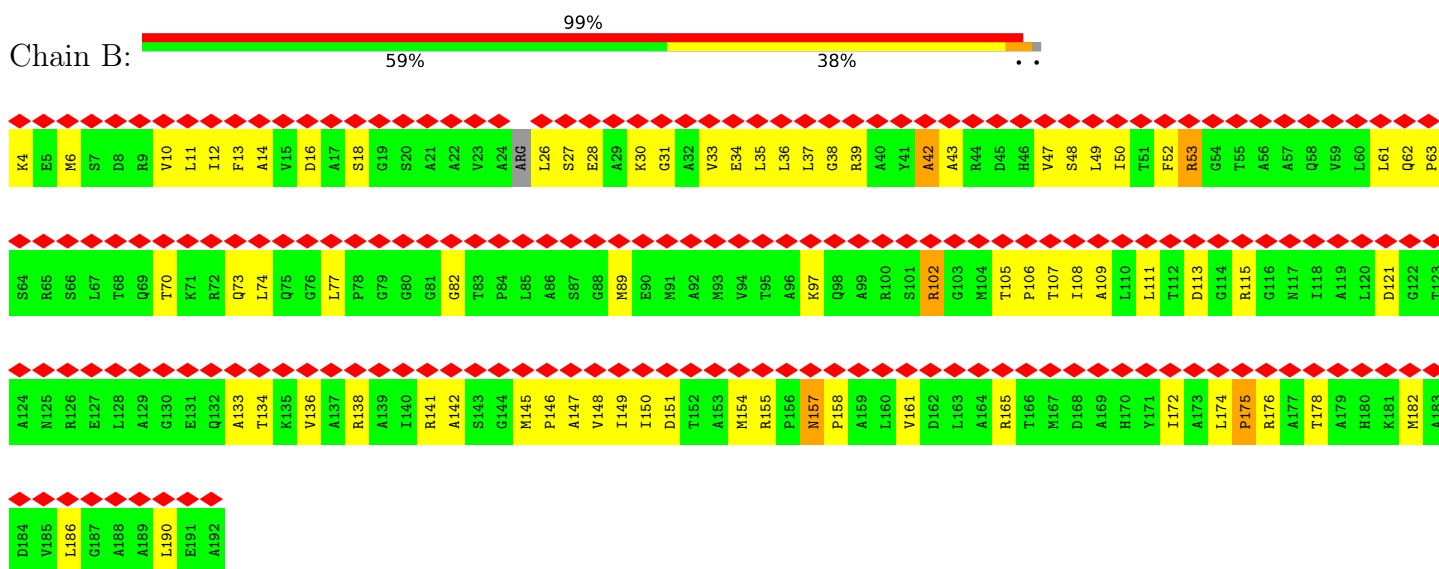
3 Residue-property plots

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.

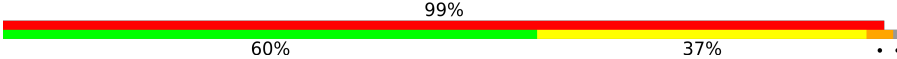
• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT



• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT

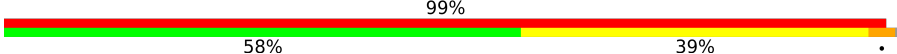


• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT

Chain C: 



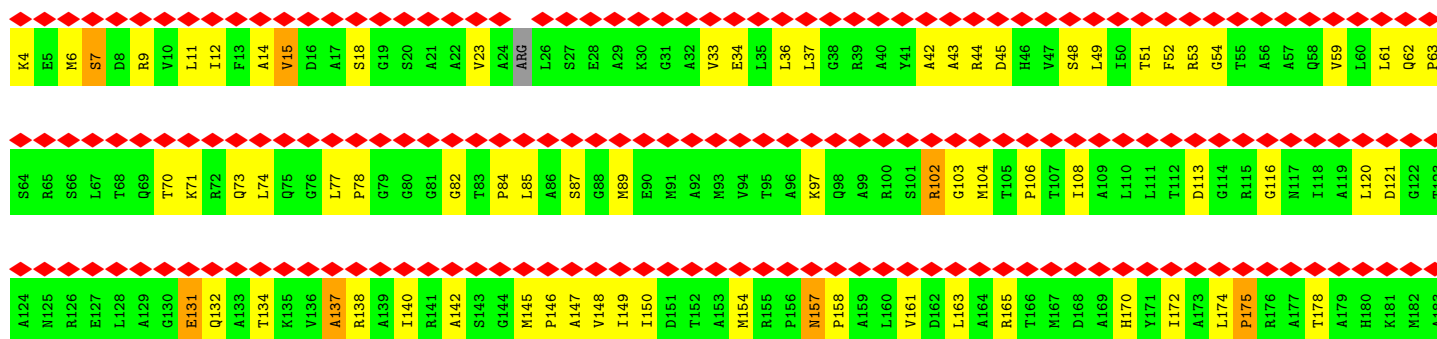
• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT

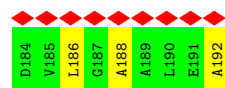
Chain D: 



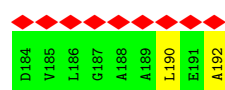
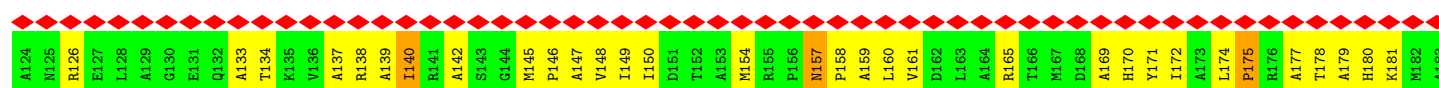
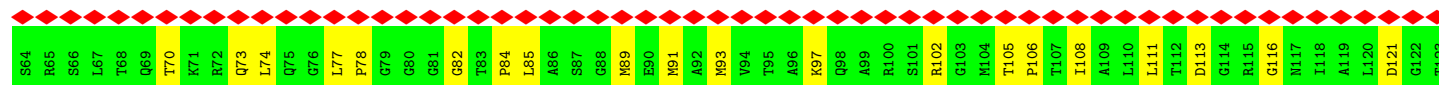
• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT

Chain E: 

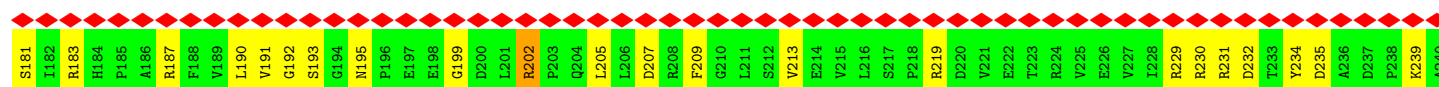
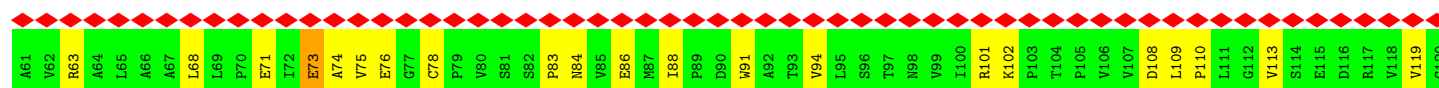




• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT

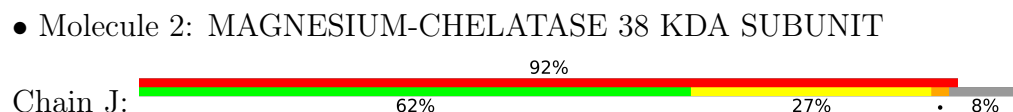
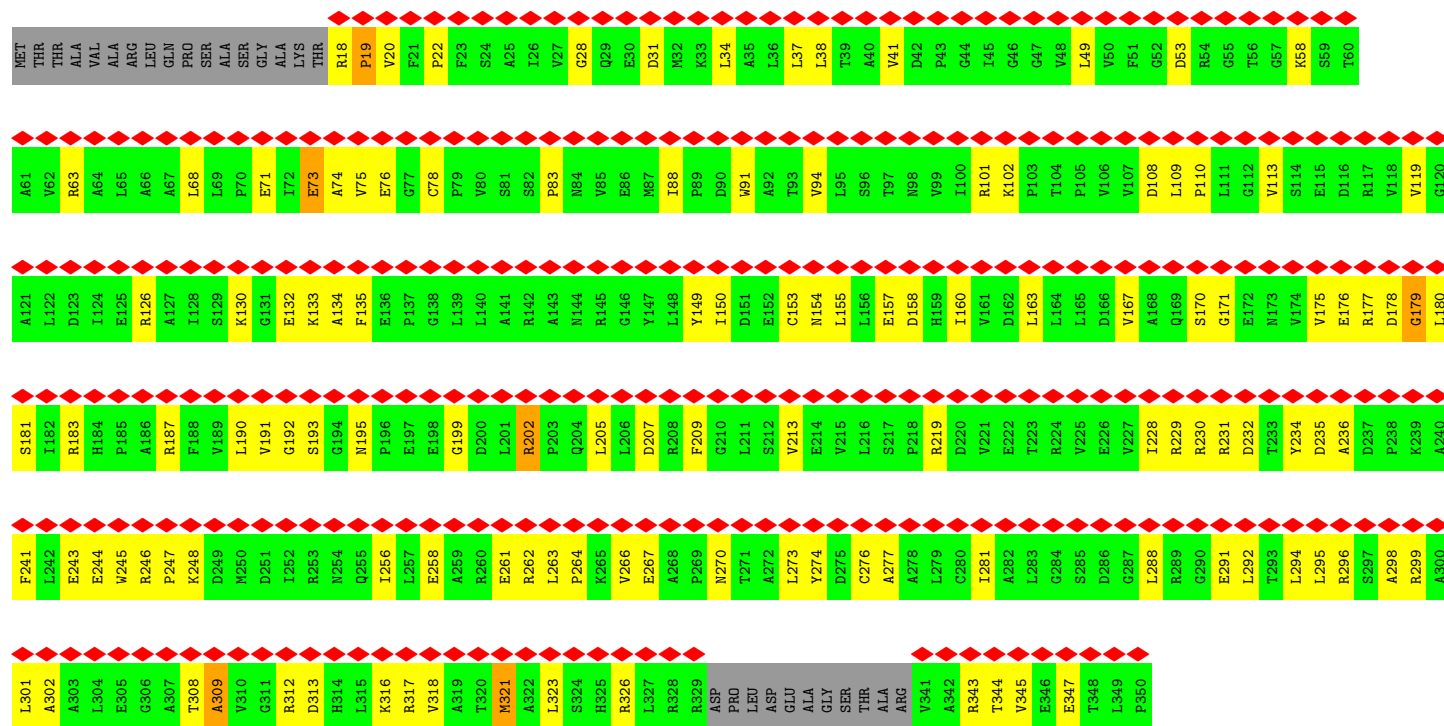
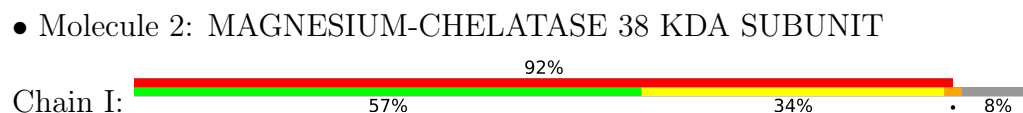
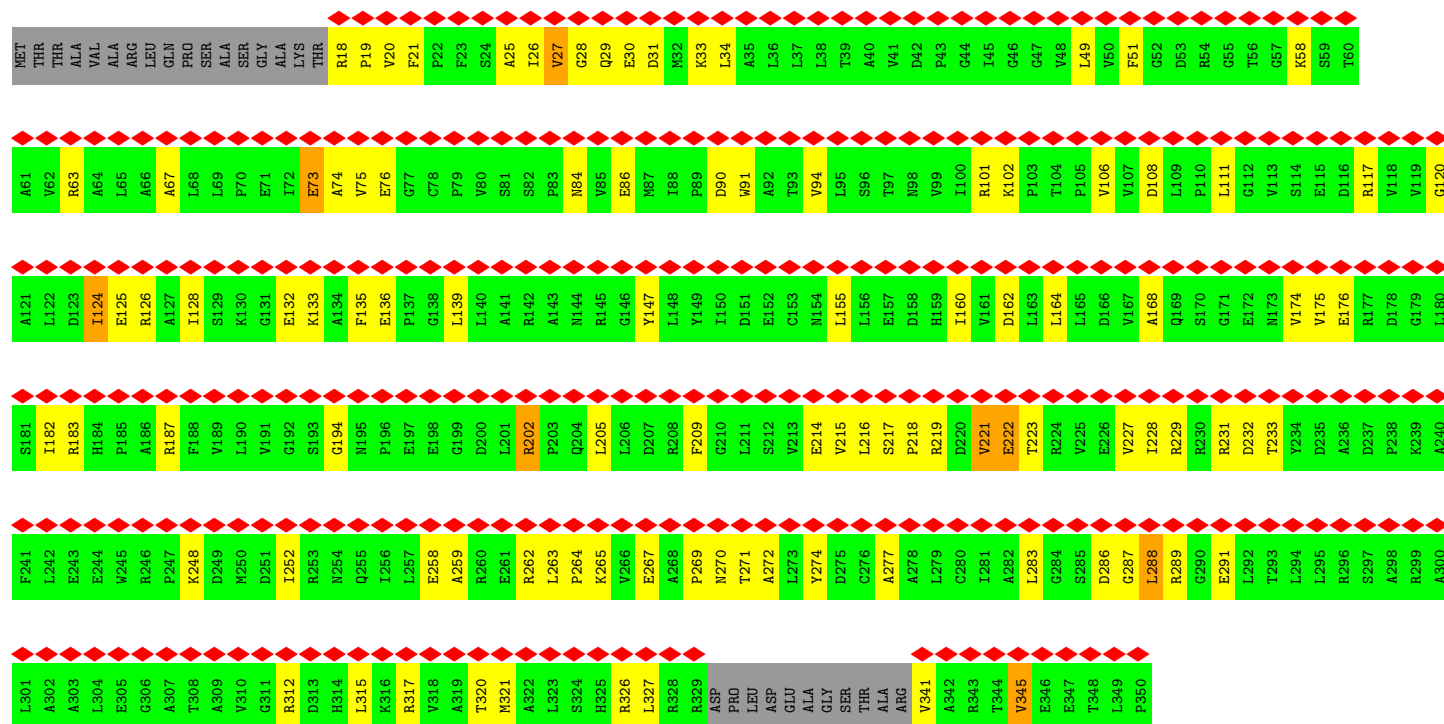


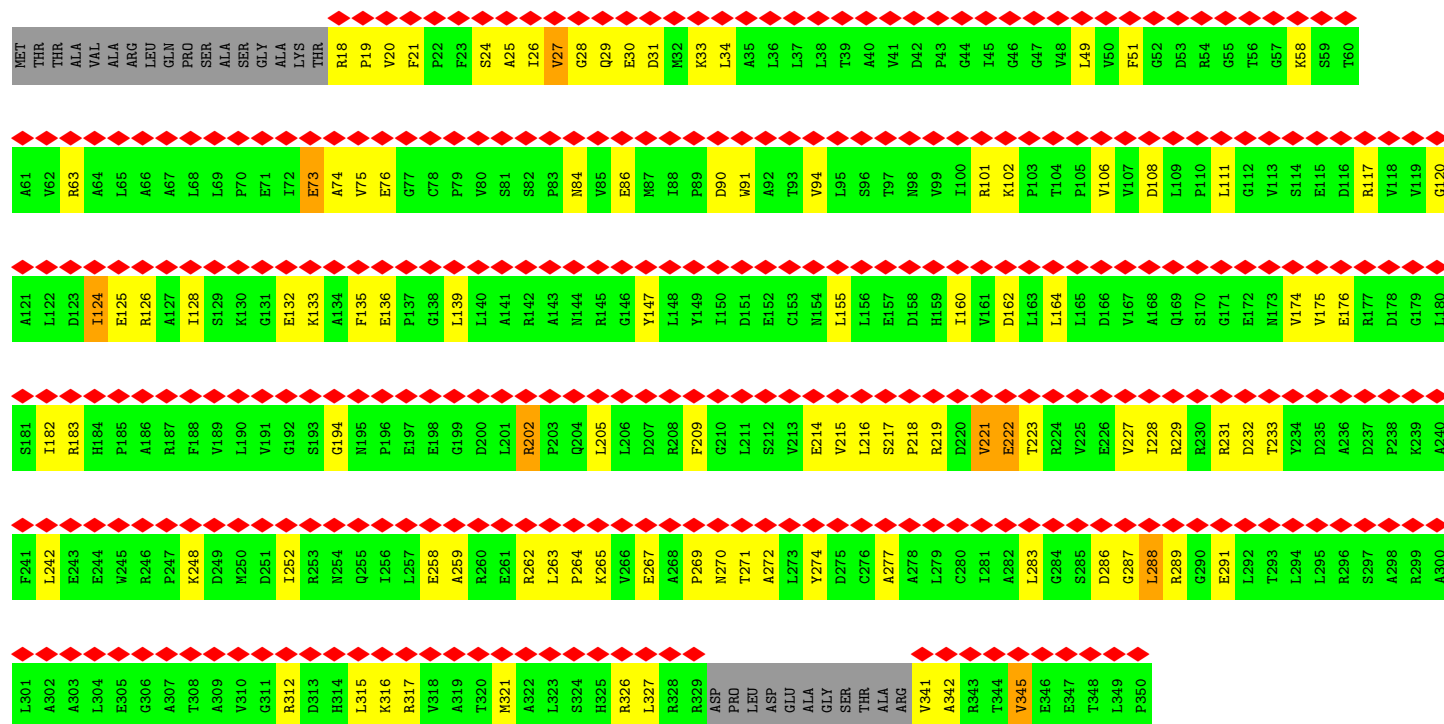
• Molecule 2: MAGNESIUM-CHELATASE 38 KDA SUBUNIT



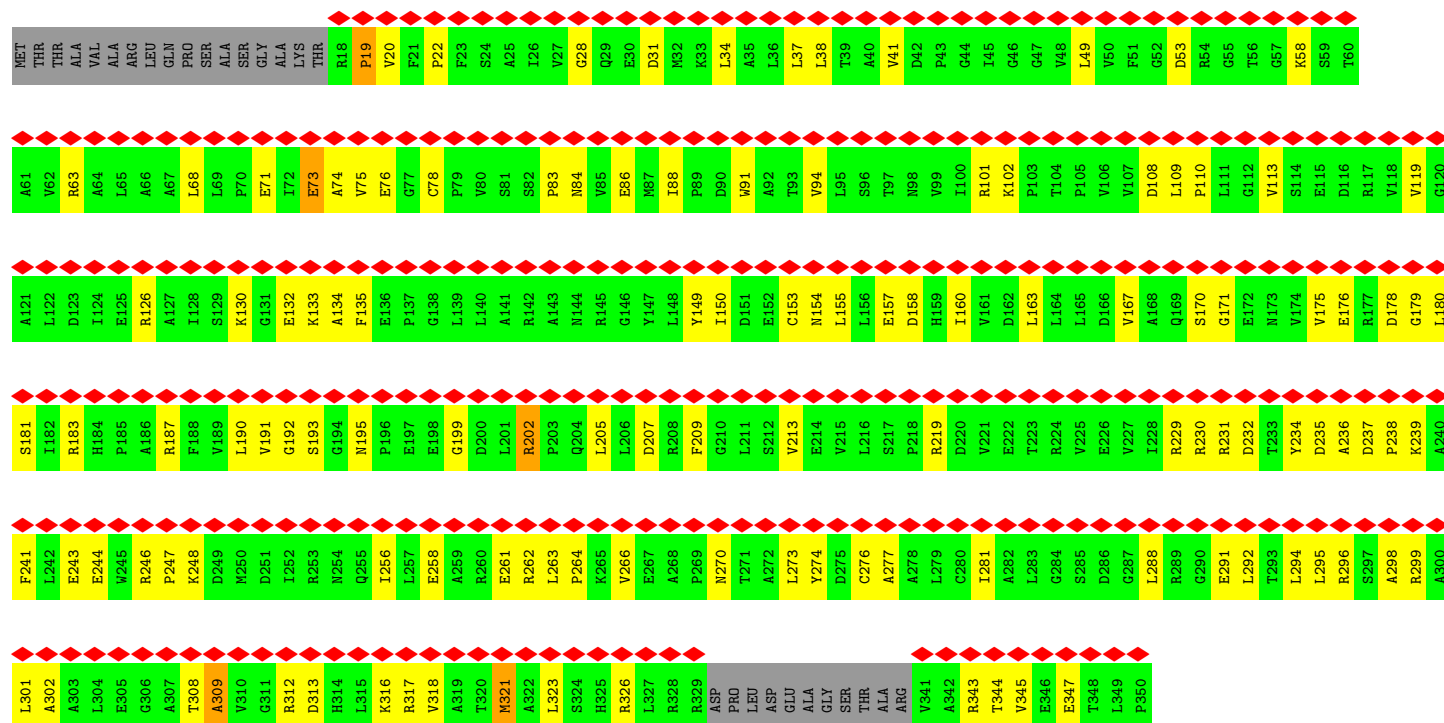
• Molecule 2: MAGNESIUM-CHELATASE 38 KDA SUBUNIT



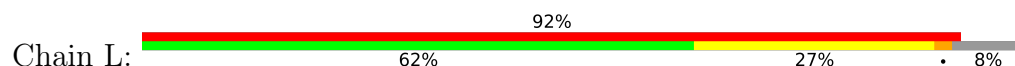




• Molecule 2: MAGNESIUM-CHELATASE 38 KDA SUBUNIT



• Molecule 2: MAGNESIUM-CHELATASE 38 KDA SUBUNIT



MET	THR	ALA	VAL	ALA	ARG	LEU	GLN	PRO	SER	ALA	SER	GLY	ALA	LYS	THR	R18	P19	V20	F21	P22	F23	S24	A25	I26	V27	G28	Q29	E30	D31	M32	K33	L34	A35	L36	L37	L38	T39	A40	V41	D42	P43	G44	I45	G46	G47	V48	L49	V50	F51	G52	D53	R54	G55	T56	G57	K58	S59	T60	
A61	V62	R63	A64	L65	A66	A67	L68	L69	P70	E71	I72	E73	A74	V75	E76	G77	C78	P79	V80	S81	S82	P83	N84	V85	E86	H87	I88	P89	D90	W91	A92	T93	V94	L95	S96	T97	N98	V99	I100	R101	K102	P103	T104	P105	V106	V107	D108	L109	P110	L111	G112	V113	S114	E115	D116	R117	V118	V119	G120
A121	L122	D123	I124	E125	R126	A127	I128	S129	K130	G131	E132	K133	A134	F135	E136	P137	G138	L139	L140	A141	R142	A143	N144	R145	G146	Y147	L148	Y149	I150	D151	E152	C153	N154	L155	L156	E157	D158	H159	I160	V161	D162	L163	L164	L165	D166	V167	A168	Q169	S170	G171	E172	N173	V174	V175	E176	R177	D178	G179	L180
S181	I182	R183	H184	P185	A186	R187	F188	V189	L190	V191	G192	S193	G194	M195	P196	E197	E198	G199	D200	L201	R202	P203	Q204	L205	L206	D207	R208	P209	Q210	L211	S212	V213	E214	V215	L216	S217	P218	R219	D220	V221	E222	T223	R224	V225	E226	V227	T228	R229	R230	R231	D232	T233	Y234	D235	A236	D237	P238	K239	A240
F241	L242	E243	E244	W245	R246	P247	K248	D249	M250	D251	I252	R253	N254	Q255	I256	L257	E258	A259	R260	E261	R262	L263	P264	K265	V266	E267	A268	P269	N270	T271	A272	L273	Y274	D275	C276	A277	A278	L279	C280	I281	A282	L283	G284	S285	D286	G287	L288	R289	Q290	E291	L292	T293	L294	L295	R296	S297	A298	R299	A300
L301	A302	A303	L304	E305	G306	A307	T308	A309	V310	G311	R312	D313	H314	L315	K316	R317	V318	A319	T320	N321	A322	L323	S324	H325	R326	L327	R328	R329	ASP	PRO	LEU	ASP	GLU	ALA	GLY	SER	THR	ALA	ARG	V341	A342	R343	T344	V345	E346	E347	T348	L349	P350										

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	29400	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	JEOL 2010F	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	60000	Depositor
Image detector	Not provided	
Maximum map value	0.077	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	186.4, 186.4, 186.4	wwPDB
Map dimensions	80, 80, 80	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	2.33, 2.33, 2.33	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	0.32	0/1370	0.80	0/1850
1	B	0.32	0/1370	0.80	0/1850
1	C	0.32	0/1370	0.80	0/1850
1	D	0.33	0/1370	0.82	0/1850
1	E	0.33	0/1370	0.80	0/1850
1	F	0.32	0/1370	0.80	0/1850
2	G	0.32	0/2495	0.80	0/3388
2	H	0.31	0/2495	0.80	2/3388 (0.1%)
2	I	0.32	0/2495	0.80	0/3388
2	J	0.31	0/2495	0.80	2/3388 (0.1%)
2	K	0.32	0/2495	0.80	0/3388
2	L	0.31	0/2495	0.80	2/3388 (0.1%)
All	All	0.32	0/23190	0.80	6/31428 (0.0%)

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(°)
2	J	202	ARG	CA-C-N	5.05	124.83	119.28
2	J	202	ARG	C-N-CA	5.05	124.83	119.28
2	H	202	ARG	CA-C-N	5.03	124.81	119.28
2	H	202	ARG	C-N-CA	5.03	124.81	119.28
2	L	202	ARG	CA-C-N	5.02	124.80	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1357	0	1409	50	0
1	B	1357	0	1409	60	0
1	C	1357	0	1409	57	0
1	D	1357	0	1409	59	0
1	E	1357	0	1409	50	0
1	F	1357	0	1409	55	0
2	G	2458	0	2507	189	0
2	H	2458	0	2503	172	0
2	I	2458	0	2507	178	0
2	J	2458	0	2505	182	0
2	K	2458	0	2507	187	0
2	L	2458	0	2504	186	0
All	All	22890	0	23487	1044	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 23.

The worst 5 of 1044 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)
2:J:321:MET:SD	2:K:232:ASP:HB2	1.41	1.58
2:G:229:ARG:HH12	2:L:317:ARG:CZ	1.11	1.57
2:G:232:ASP:CG	2:L:317:ARG:HH22	1.10	1.57
2:G:229:ARG:CZ	2:L:317:ARG:NH1	1.69	1.56
2:G:295:LEU:HD22	2:H:232:ASP:C	1.05	1.47

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	184/189 (97%)	138 (75%)	33 (18%)	13 (7%)	1	11
1	B	184/189 (97%)	133 (72%)	42 (23%)	9 (5%)	1	16
1	C	184/189 (97%)	137 (74%)	31 (17%)	16 (9%)	0	9
1	D	184/189 (97%)	135 (73%)	37 (20%)	12 (6%)	1	12
1	E	184/189 (97%)	136 (74%)	32 (17%)	16 (9%)	0	9
1	F	184/189 (97%)	138 (75%)	30 (16%)	16 (9%)	0	9
2	G	318/350 (91%)	257 (81%)	48 (15%)	13 (4%)	2	18
2	H	318/350 (91%)	267 (84%)	42 (13%)	9 (3%)	4	24
2	I	318/350 (91%)	257 (81%)	48 (15%)	13 (4%)	2	18
2	J	318/350 (91%)	267 (84%)	42 (13%)	9 (3%)	4	24
2	K	318/350 (91%)	257 (81%)	48 (15%)	13 (4%)	2	18
2	L	318/350 (91%)	267 (84%)	42 (13%)	9 (3%)	4	24
All	All	3012/3234 (93%)	2389 (79%)	475 (16%)	148 (5%)	3	16

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	ALA
1	D	53	ARG
2	G	76	GLU
2	H	221	VAL
2	H	288	LEU

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	135/136 (99%)	135 (100%)	0	100	100
1	B	135/136 (99%)	134 (99%)	1 (1%)	76	81
1	C	135/136 (99%)	135 (100%)	0	100	100
1	D	135/136 (99%)	132 (98%)	3 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	135/136 (99%)	133 (98%)	2 (2%)	57	72
1	F	135/136 (99%)	134 (99%)	1 (1%)	76	81
2	G	264/285 (93%)	259 (98%)	5 (2%)	50	67
2	H	264/285 (93%)	262 (99%)	2 (1%)	73	80
2	I	264/285 (93%)	259 (98%)	5 (2%)	50	67
2	J	264/285 (93%)	262 (99%)	2 (1%)	73	80
2	K	264/285 (93%)	259 (98%)	5 (2%)	50	67
2	L	264/285 (93%)	262 (99%)	2 (1%)	73	80
All	All	2394/2526 (95%)	2366 (99%)	28 (1%)	61	75

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	73	GLU
2	L	124	ILE
2	I	317	ARG
2	K	317	ARG
2	I	261	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	255	GLN
2	J	154	ASN
2	I	254	ASN
2	J	173	ASN
1	E	58	GLN

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 [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-1676. These allow visual inspection of the internal detail of the map and identification of artifacts.

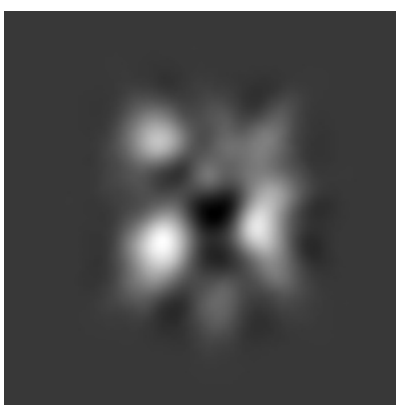
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

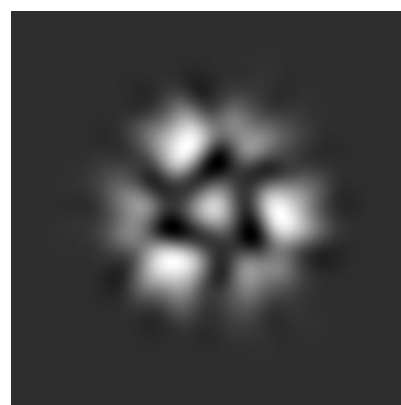
6.1.1 Primary map



X



Y

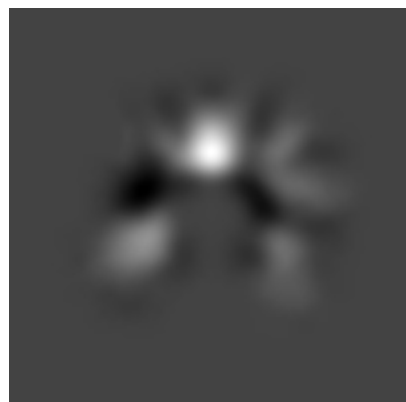


Z

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

6.2 Central slices [i](#)

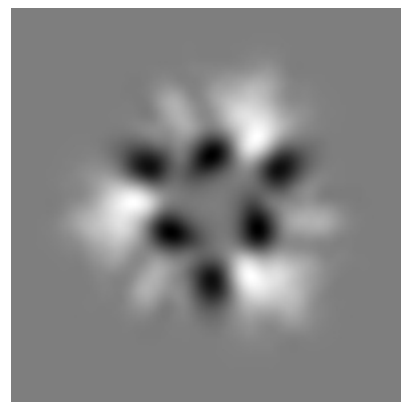
6.2.1 Primary map



X Index: 40



Y Index: 40



Z Index: 40

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: 34



Y Index: 40



Z Index: 31

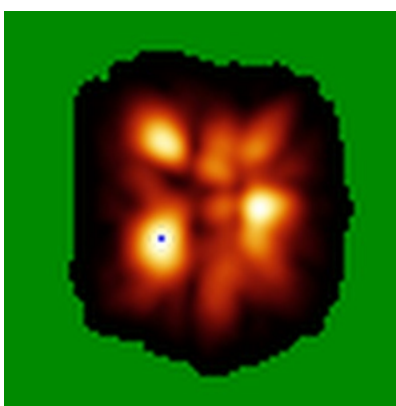
The images above show the largest variance slices of the map in three orthogonal directions.

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

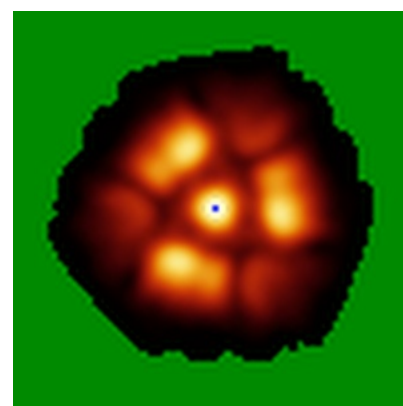
6.4.1 Primary map



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

This section was not generated.

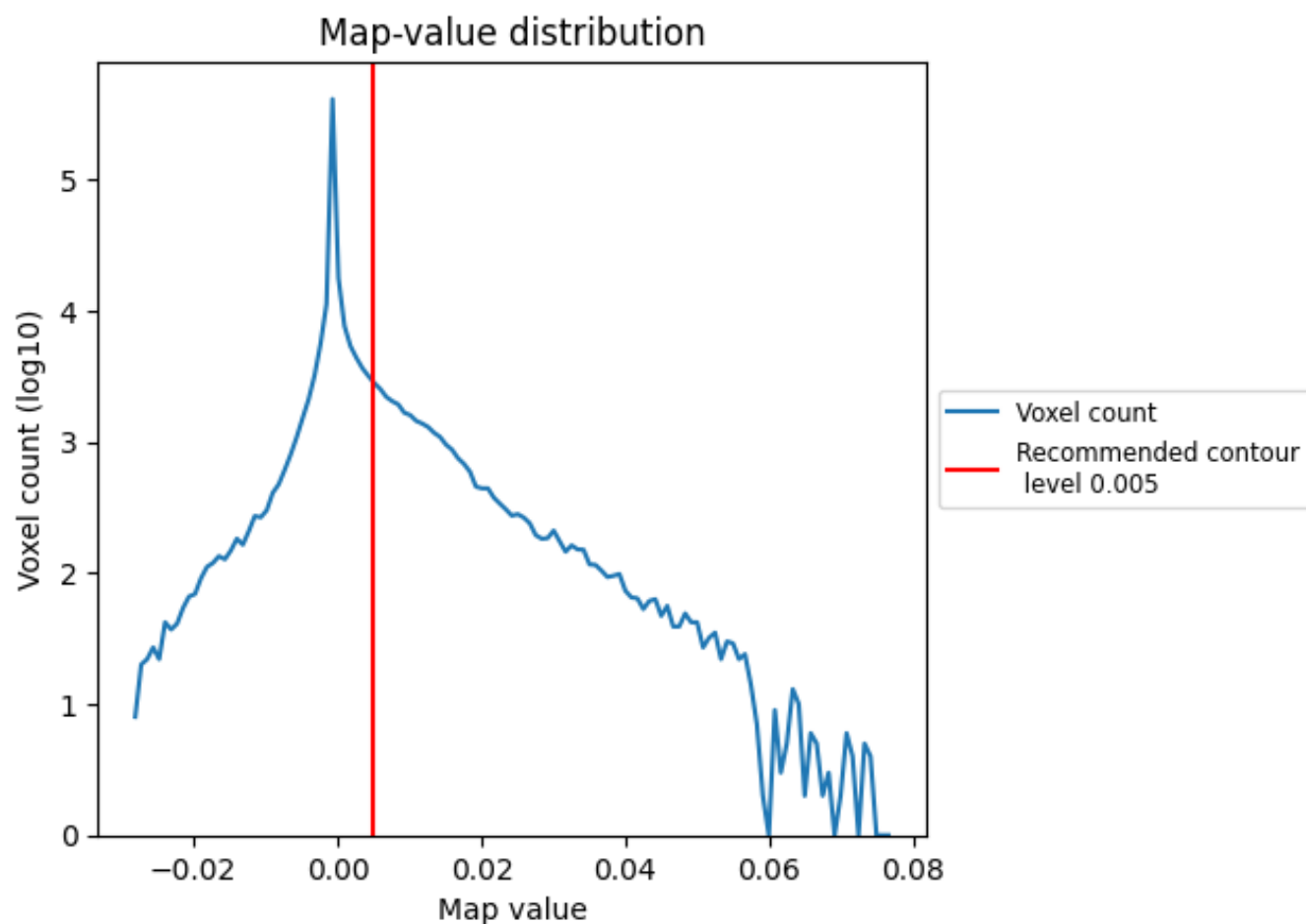
6.6 Mask visualisation

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

7 Map analysis [i](#)

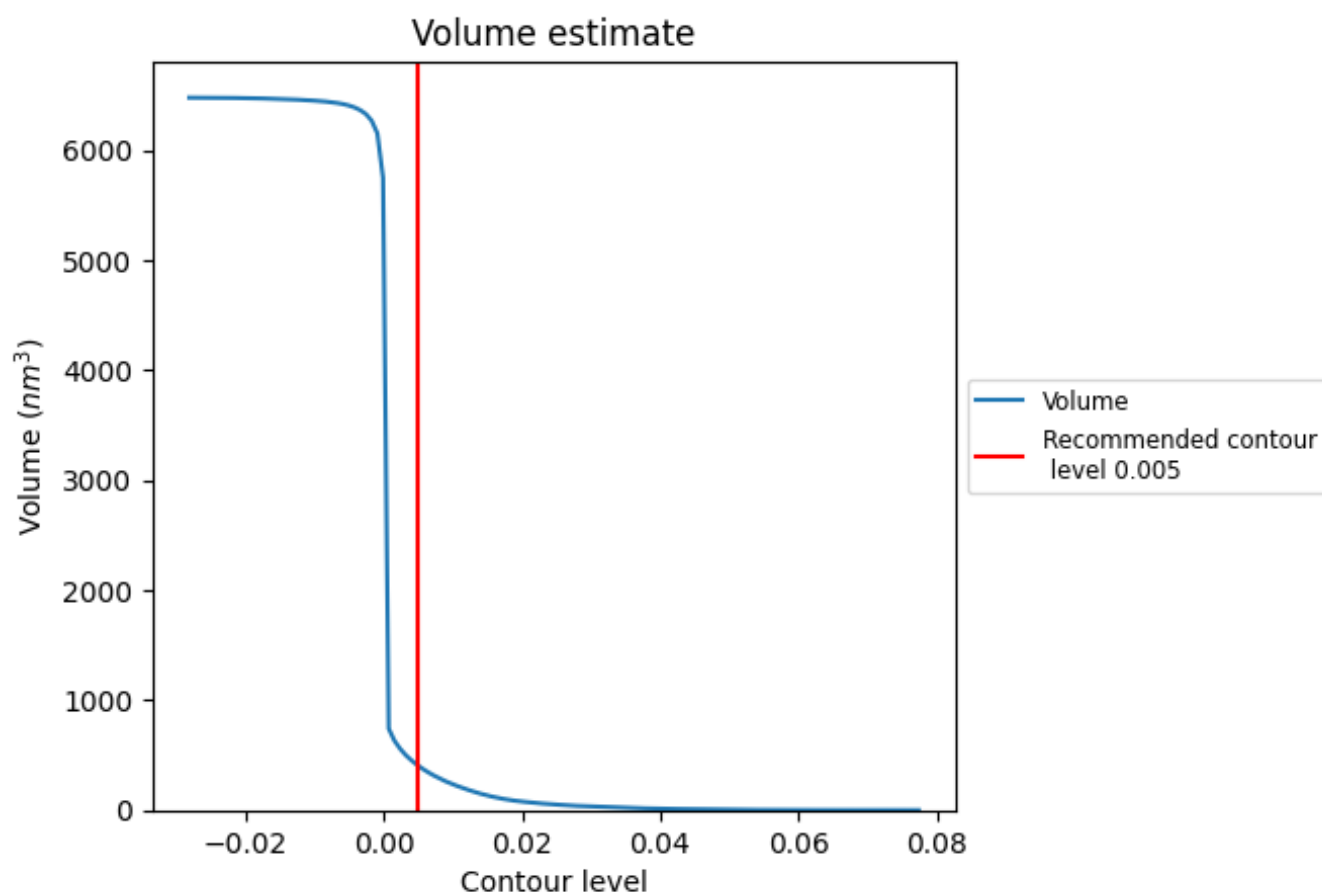
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

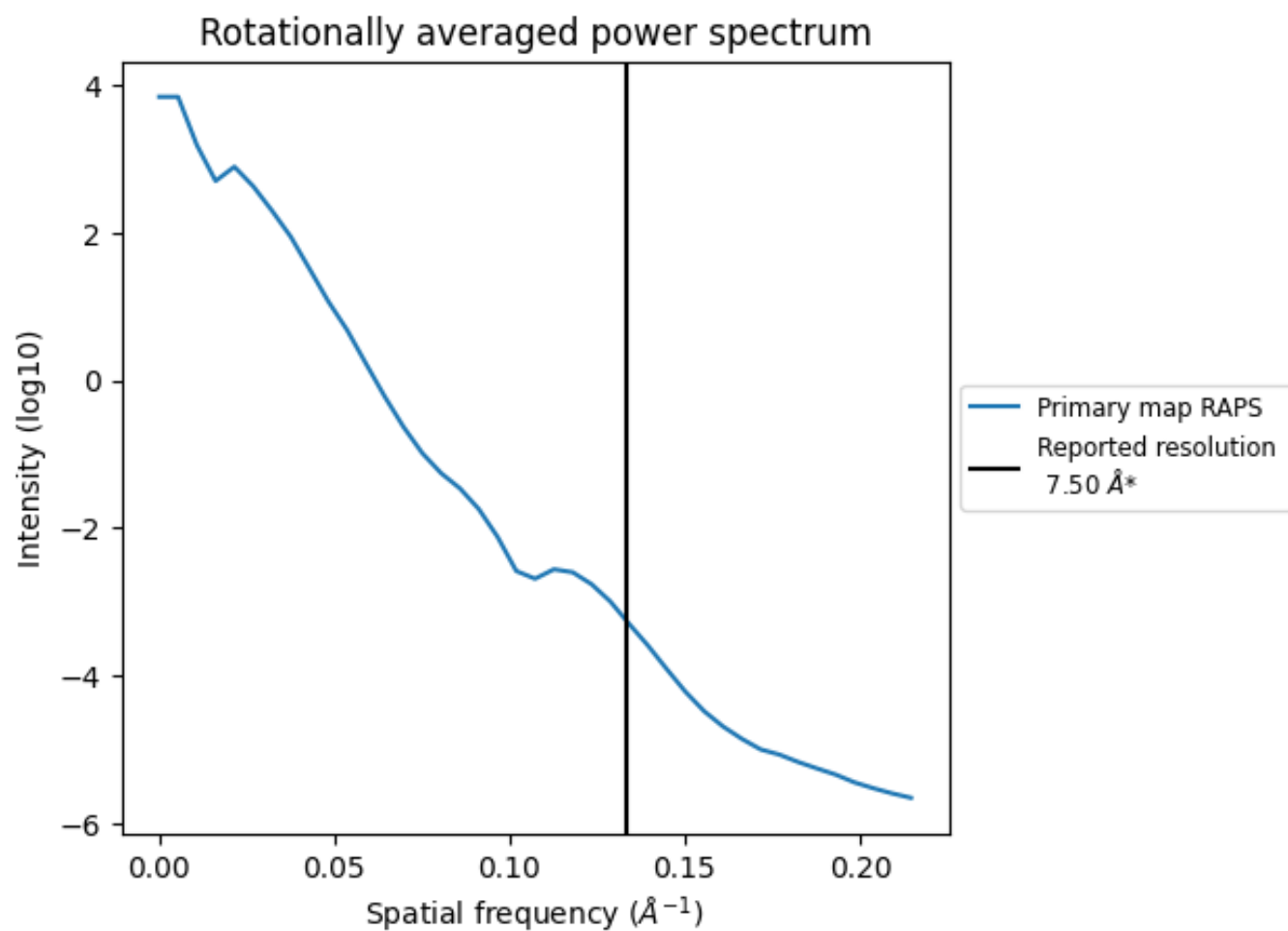
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404 nm^3 ; this corresponds to an approximate mass of 365 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 0.133 Å⁻¹

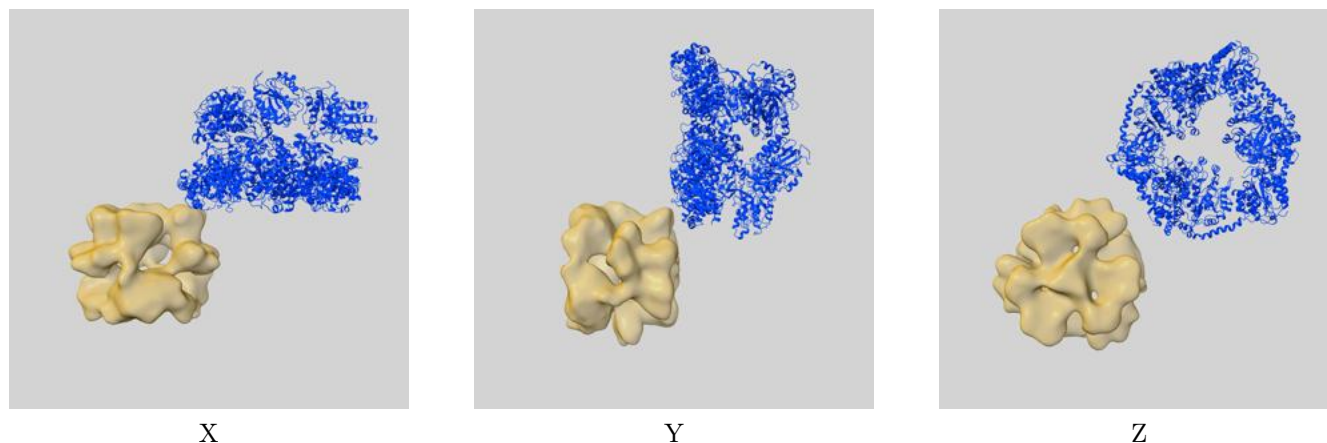
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

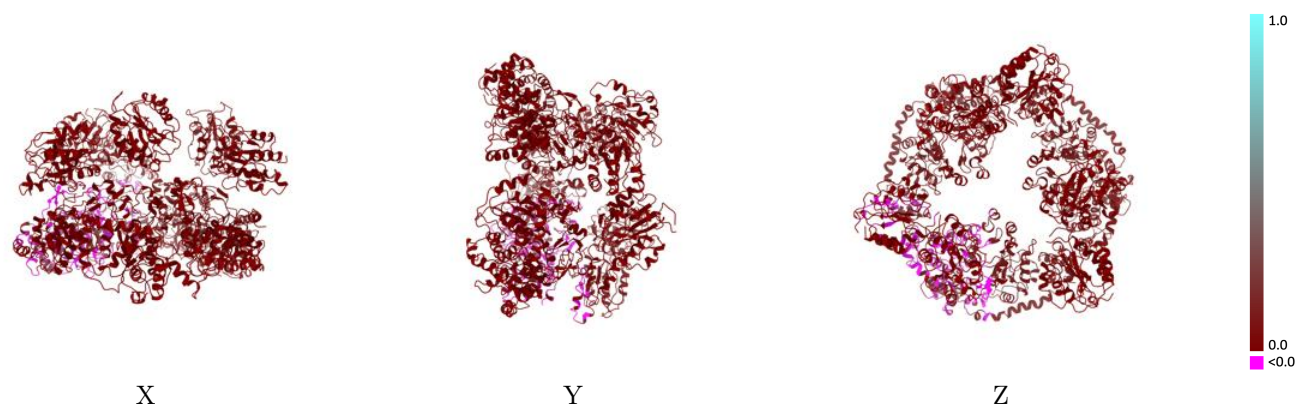
This section contains information regarding the fit between EMDB map EMD-1676 and PDB model 2X31. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



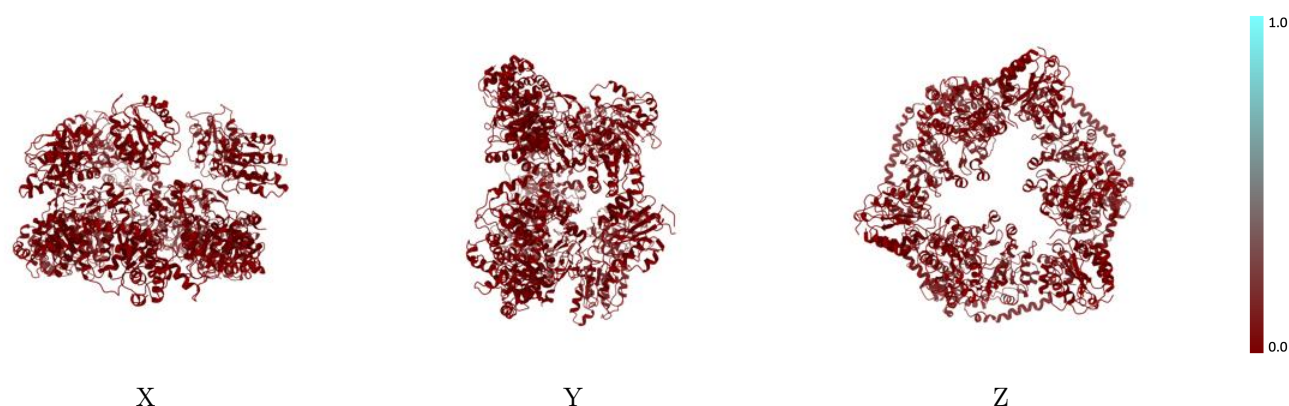
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



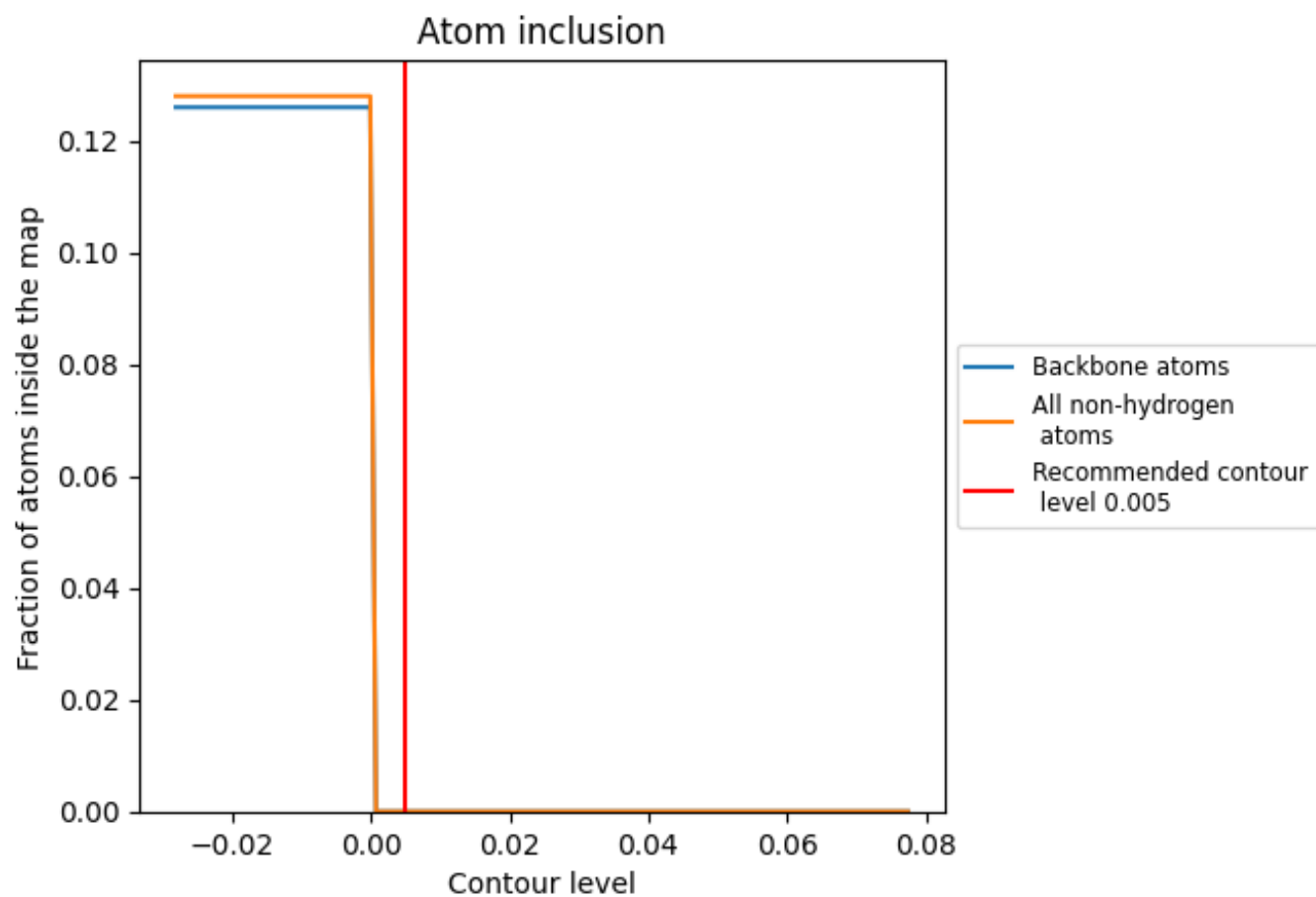
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion ⓘ



At the recommended contour level, 0% of all backbone atoms, 0% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	-0.0030
A	0.0000	0.0000
B	0.0000	0.0000
C	0.0000	-0.0070
D	0.0000	0.0000
E	0.0000	0.0000
F	0.0000	0.0000
G	0.0000	0.0000
H	0.0000	0.0000
I	0.0000	0.0000
J	0.0000	-0.0020
K	0.0000	-0.0120
L	0.0000	-0.0080

1.0

0.0

<0.0