



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:53 PM BST

PDB ID : 2X31
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 PDB ID : 1G8P

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

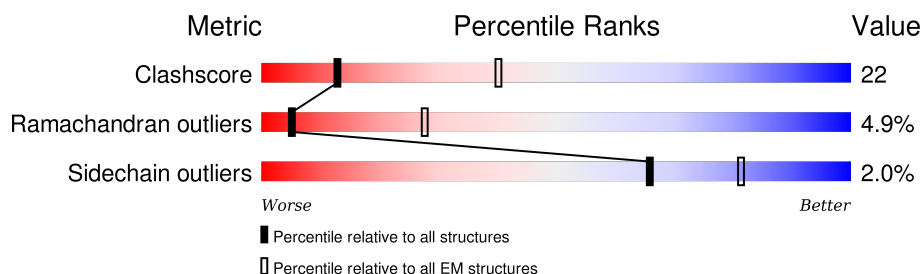
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	189	61% 35% . ..
1	B	189	58% 39% . .
1	C	189	61% 34% . .
1	D	189	58% 39% . .
1	E	189	62% 34% . .
1	F	189	56% 41% . .
2	G	350	57% 33% . 8%
2	H	350	63% 27% . 8%
2	I	350	57% 33% . 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	350	<div><div></div><div>63%</div><div>27%</div><div>• 8%</div></div>
2	K	350	<div><div></div><div>57%</div><div>34%</div><div>• 8%</div></div>
2	L	350	<div><div></div><div>64%</div><div>26%</div><div>• 8%</div></div>

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.

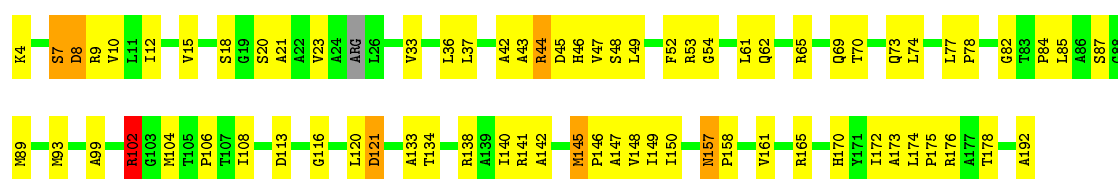
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	322	Total	C	N	O	S	0	1
			2458	1540	443	467	8		
2	H	322	Total	C	N	O	S	0	1
			2458	1540	443	467	8		
2	I	322	Total	C	N	O	S	0	1
			2458	1540	443	467	8		
2	J	322	Total	C	N	O	S	0	1
			2458	1540	443	467	8		
2	K	322	Total	C	N	O	S	0	1
			2458	1540	443	467	8		
2	L	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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

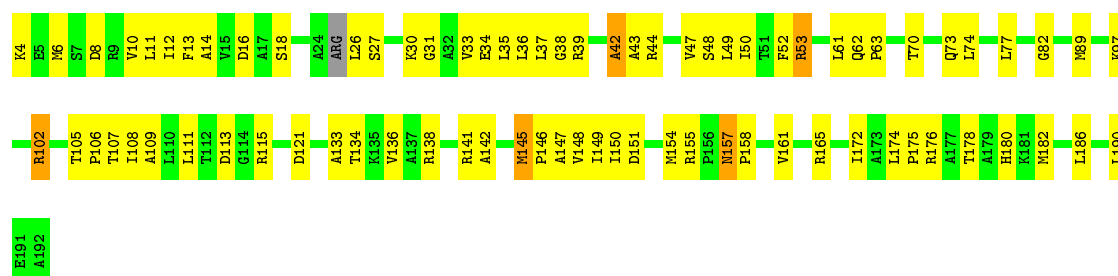
• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT

Chain A: 



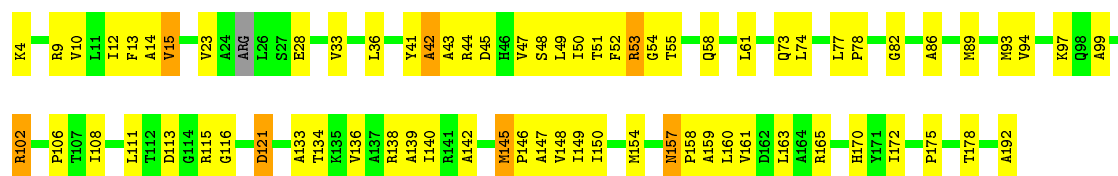
• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT

Chain B: 



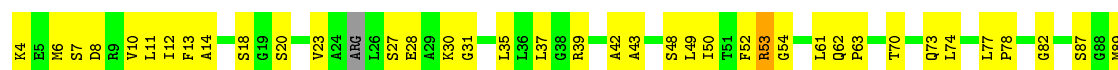
• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT

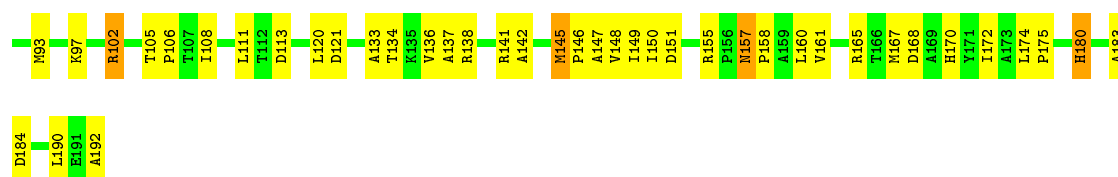
Chain C: 



• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT

Chain D: 





• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT

Chain E: 62% 34%



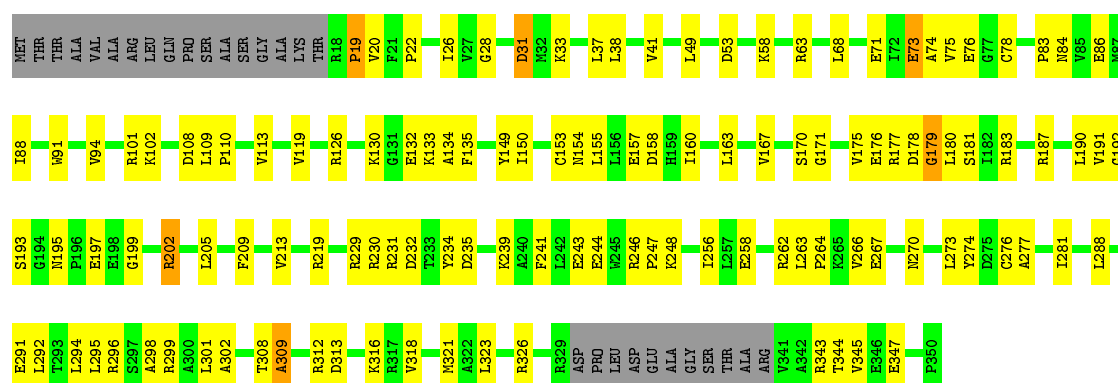
• Molecule 1: MAGNESIUM-CHELATASE 60 KDA SUBUNIT

Chain F: 56% 41%



• Molecule 2: MAGNESIUM-CHELATASE 38 KDA SUBUNIT

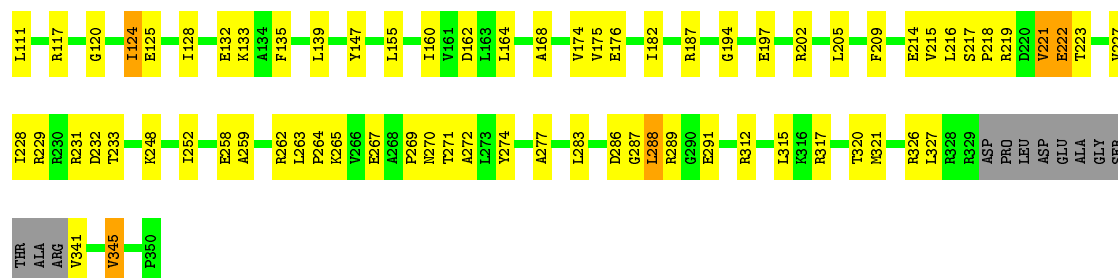
Chain G: 57% 33% 8%



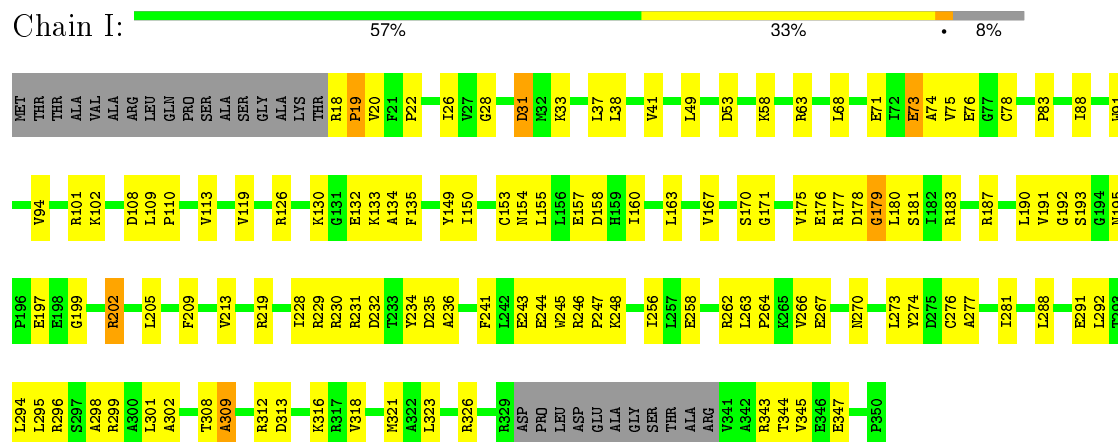
• Molecule 2: MAGNESIUM-CHELATASE 38 KDA SUBUNIT

Chain H: 63% 27% 8%

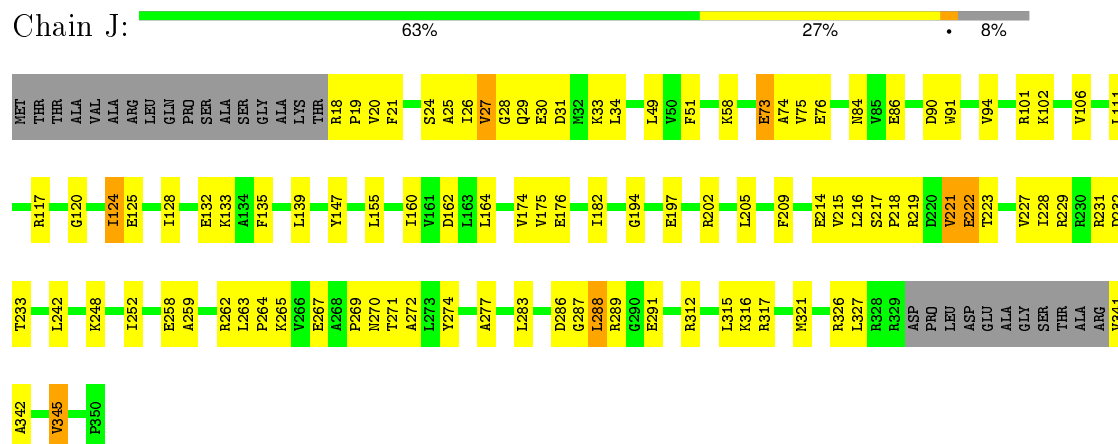




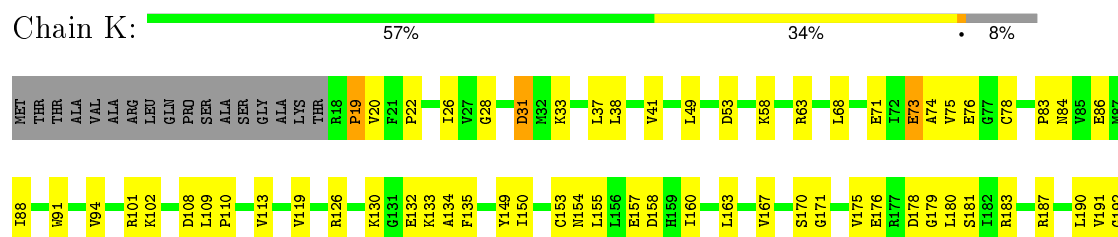
• Molecule 2: MAGNESIUM-CHELATASE 38 KDA SUBUNIT



• Molecule 2: MAGNESIUM-CHELATASE 38 KDA SUBUNIT



• Molecule 2: MAGNESIUM-CHELATASE 38 KDA SUBUNIT



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 2010F	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1	Depositor
Maximum defocus (nm)	5.5	Depositor
Magnification	60000	Depositor
Image detector	Not provided	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 >2	RMSZ	# Z >2
1	A	0.28	0/1370	0.51	0/1850
1	B	0.27	0/1370	0.51	0/1850
1	C	0.28	0/1370	0.51	0/1850
1	D	0.27	0/1370	0.51	0/1850
1	E	0.28	0/1370	0.51	0/1850
1	F	0.28	0/1370	0.50	0/1850
2	G	0.27	0/2495	0.49	0/3388
2	H	0.27	0/2495	0.49	0/3388
2	I	0.27	0/2495	0.49	0/3388
2	J	0.27	0/2495	0.49	0/3388
2	K	0.27	0/2495	0.49	0/3388
2	L	0.27	0/2495	0.49	0/3388
All	All	0.27	0/23190	0.50	0/31428

There are no bond length outliers.

There are no bond angle outliers.

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	46	0
1	B	1357	0	1409	58	0
1	C	1357	0	1409	54	0
1	D	1357	0	1409	55	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1357	0	1409	44	0
1	F	1357	0	1409	54	0
2	G	2458	0	2507	187	0
2	H	2458	0	2503	166	0
2	I	2458	0	2507	173	0
2	J	2458	0	2505	178	0
2	K	2458	0	2507	183	0
2	L	2458	0	2504	180	0
All	All	22890	0	23487	1003	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 22.

The worst 5 of 1003 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:229:ARG:CZ	2:L:317:ARG:NH1	1.69	1.56
2:G:232:ASP:CG	2:L:317:ARG:HH22	1.10	1.52
2:H:341:VAL:CG2	2:I:236:ALA:CB	1.94	1.45

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	22
1	B	184/189 (97%)	133 (72%)	42 (23%)	9 (5%)	3	31
1	C	184/189 (97%)	137 (74%)	31 (17%)	16 (9%)	1	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	184/189 (97%)	135 (73%)	37 (20%)	12 (6%)	1	25
1	E	184/189 (97%)	136 (74%)	32 (17%)	16 (9%)	1	17
1	F	184/189 (97%)	138 (75%)	30 (16%)	16 (9%)	1	17
2	G	318/350 (91%)	257 (81%)	48 (15%)	13 (4%)	3	35
2	H	318/350 (91%)	267 (84%)	42 (13%)	9 (3%)	6	44
2	I	318/350 (91%)	257 (81%)	48 (15%)	13 (4%)	3	35
2	J	318/350 (91%)	267 (84%)	42 (13%)	9 (3%)	6	44
2	K	318/350 (91%)	257 (81%)	48 (15%)	13 (4%)	3	35
2	L	318/350 (91%)	267 (84%)	42 (13%)	9 (3%)	6	44
All	All	3012/3234 (93%)	2389 (79%)	475 (16%)	148 (5%)	5	31

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%)	130 (96%)	5 (4%)	41	73
1	B	135/136 (99%)	131 (97%)	4 (3%)	48	77
1	C	135/136 (99%)	133 (98%)	2 (2%)	72	88
1	D	135/136 (99%)	130 (96%)	5 (4%)	41	73
1	E	135/136 (99%)	131 (97%)	4 (3%)	48	77
1	F	135/136 (99%)	132 (98%)	3 (2%)	60	83
2	G	264/285 (93%)	259 (98%)	5 (2%)	65	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	264/285 (93%)	261 (99%)	3 (1%)	80	91
2	I	264/285 (93%)	259 (98%)	5 (2%)	65	86
2	J	264/285 (93%)	261 (99%)	3 (1%)	80	91
2	K	264/285 (93%)	259 (98%)	5 (2%)	65	86
2	L	264/285 (93%)	261 (99%)	3 (1%)	80	91
All	All	2394/2526 (95%)	2347 (98%)	47 (2%)	66	85

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	121	ASP
2	G	202	ARG
2	K	344	THR
2	G	31	ASP
2	G	344	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	173	ASN
2	H	255	GLN
2	K	154	ASN
2	G	154	ASN
2	J	255	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 ⓘ

There are no carbohydrates 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.