



wwPDB EM Validation Summary Report ⓘ

Oct 15, 2024 – 12:08 PM JST

PDB ID : 8IZ8
EMDB ID : EMD-35835
Title : cryo EM structure of apo hMRP4
Authors : Liu, Z.M.; Huang, Y.
Deposited on : 2023-04-06
Resolution : 3.13 Å(reported)

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

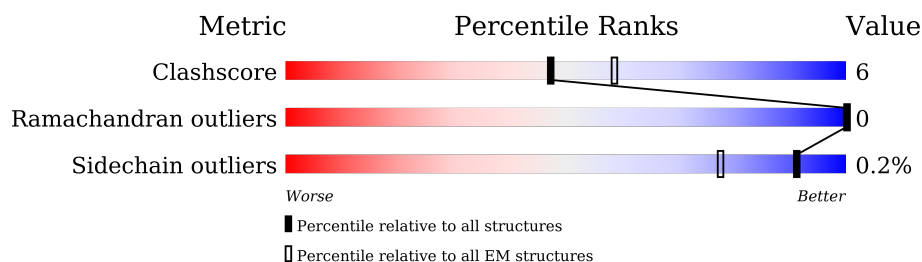
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 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	210492	15764
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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1357	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 9805 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 ATP-binding cassette sub-family C member 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1230	Total	C	N	O	S	0	0
			9805	6366	1645	1750	44		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1326	LEU	-	expression tag	UNP O15439
A	1327	GLU	-	expression tag	UNP O15439
A	1328	GLY	-	expression tag	UNP O15439
A	1329	GLY	-	expression tag	UNP O15439
A	1330	GLY	-	expression tag	UNP O15439
A	1331	SER	-	expression tag	UNP O15439
A	1332	GLY	-	expression tag	UNP O15439
A	1333	GLY	-	expression tag	UNP O15439
A	1334	GLY	-	expression tag	UNP O15439
A	1335	SER	-	expression tag	UNP O15439
A	1336	ASP	-	expression tag	UNP O15439
A	1337	TYR	-	expression tag	UNP O15439
A	1338	LYS	-	expression tag	UNP O15439
A	1339	ASP	-	expression tag	UNP O15439
A	1340	HIS	-	expression tag	UNP O15439
A	1341	ASP	-	expression tag	UNP O15439
A	1342	GLY	-	expression tag	UNP O15439
A	1343	ASP	-	expression tag	UNP O15439
A	1344	TYR	-	expression tag	UNP O15439
A	1345	LYS	-	expression tag	UNP O15439
A	1346	ASP	-	expression tag	UNP O15439
A	1347	HIS	-	expression tag	UNP O15439
A	1348	ASP	-	expression tag	UNP O15439
A	1349	ILE	-	expression tag	UNP O15439
A	1350	ASP	-	expression tag	UNP O15439
A	1351	TYR	-	expression tag	UNP O15439
A	1352	LYS	-	expression tag	UNP O15439
A	1353	ASP	-	expression tag	UNP O15439

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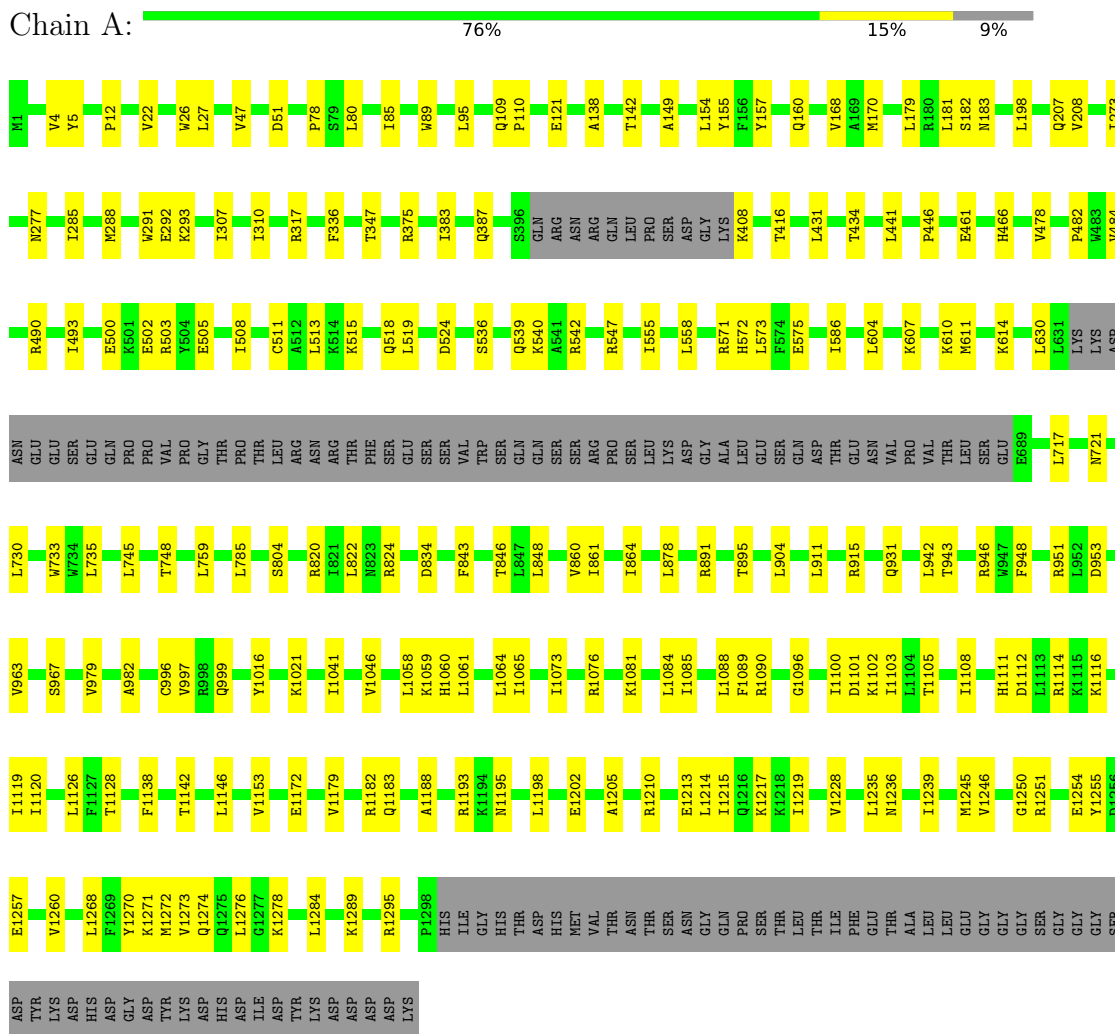
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1354	ASP	-	expression tag	UNP O15439
A	1355	ASP	-	expression tag	UNP O15439
A	1356	ASP	-	expression tag	UNP O15439
A	1357	LYS	-	expression tag	UNP O15439

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. 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: ATP-binding cassette sub-family C member 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	203347	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.23	0/10015	0.38	0/13575

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

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	9805	0	10058	116	0
All	All	9805	0	10058	116	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 6.

The worst 5 of 116 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)
1:A:85:ILE:O	1:A:89:TRP:HB3	1.84	0.78
1:A:1058:LEU:HG	1:A:1061:LEU:HD11	1.69	0.73
1:A:408:LYS:HB2	1:A:586:ILE:HD11	1.72	0.71
1:A:157:TYR:HB2	1:A:946:ARG:HG3	1.75	0.68
1:A:1100:ILE:HG22	1:A:1105:THR:HG22	1.77	0.67

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	1224/1357 (90%)	1201 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1071/1184 (90%)	1069 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1059	LYS
1	A	1295	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1290	GLN
1	A	1225	HIS
1	A	931	GLN

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Mol	Chain	Res	Type
1	A	845	GLN
1	A	1183	GLN

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.