



wwPDB EM Validation Summary Report ⓘ

Oct 16, 2024 – 01:21 AM JST

PDB ID : 8JY5
EMDB ID : EMD-36720
Title : Cryo-EM structure of human ABC transporter ABCC2 in apo" state
Authors : Mao, Y.X.; Chen, Z.P.; Wang, L.; Hou, W.T.; Chen, Y.X.; Zhou, C.Z.
Deposited on : 2023-07-03
Resolution : 4.17 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

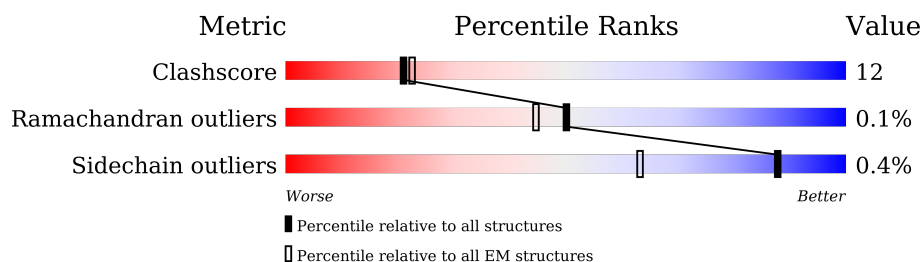
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.17 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	1565	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11511 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1457	Total	C	N	O	S	0	0
			11511	7448	1908	2097	58		

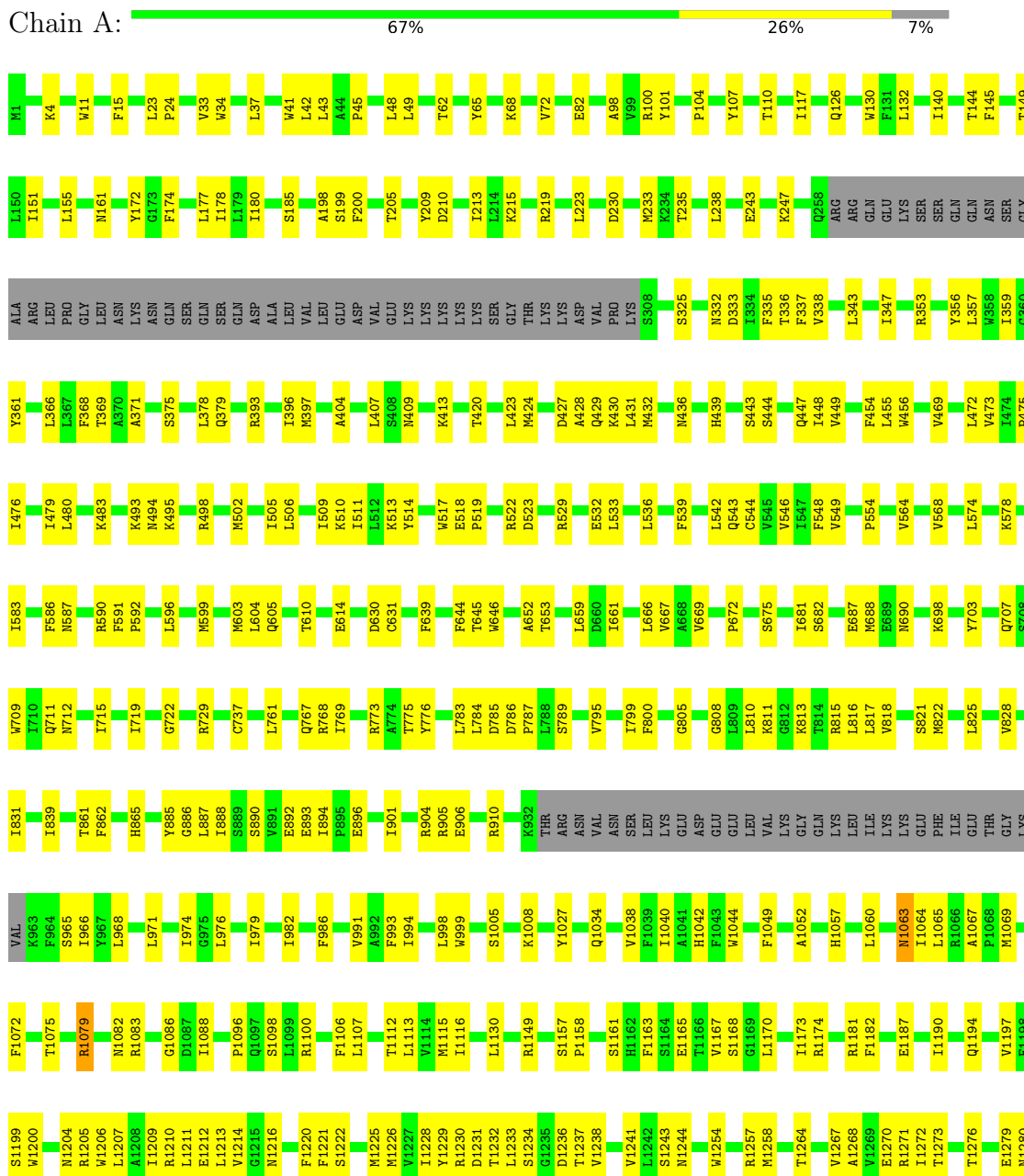
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1546	LEU	-	expression tag	UNP Q92887
A	1547	GLU	-	expression tag	UNP Q92887
A	1548	ASP	-	expression tag	UNP Q92887
A	1549	TYR	-	expression tag	UNP Q92887
A	1550	LYS	-	expression tag	UNP Q92887
A	1551	ASP	-	expression tag	UNP Q92887
A	1552	ASP	-	expression tag	UNP Q92887
A	1553	ASP	-	expression tag	UNP Q92887
A	1554	ASP	-	expression tag	UNP Q92887
A	1555	LYS	-	expression tag	UNP Q92887
A	1556	VAL	-	expression tag	UNP Q92887
A	1557	GLU	-	expression tag	UNP Q92887
A	1558	HIS	-	expression tag	UNP Q92887
A	1559	HIS	-	expression tag	UNP Q92887
A	1560	HIS	-	expression tag	UNP Q92887
A	1561	HIS	-	expression tag	UNP Q92887
A	1562	HIS	-	expression tag	UNP Q92887
A	1563	HIS	-	expression tag	UNP Q92887
A	1564	HIS	-	expression tag	UNP Q92887
A	1565	HIS	-	expression tag	UNP Q92887

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. 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 2



HIS	Q1441	E1281
HIS	Q1442	W1284
HIS	Q1443	L1300
HIS	L1444	Q1301
HIS	L1445	F1302
HIS	Q1446	Y1305
HIS	L1447	R1308
	R1453	Y1309
	L1460	L1315
	D1461	T1316
	E1462	L1320
	A1463	T1321
	T1464	C1322
	A1465	D1323
	A1466	I1324
	A1467	K1329
	D1468	I1330
	T1475	G1331
	T1477	V1332
	I1476	N1345
	T1478	C1346
	I1479	R1349
	V1488	I1350
	I1489	I1368
	T1490	H1371
	I1491	L1377
	I1498	P1384
	K1503	G1389
	I1512	R1392
	G1536	L1395
	I15	D1396
	GLU	P1397
	ASN	F1398
	VAL	N1399
	ASN	N1400
	THR	L1403
	SER	L1415
	LYS	V1430
	PHE	L1439
	LEU	G1440
	GLU	T1441
	ASP	T1442
	TVR	T1443
	LYS	T1444
	ASP	T1445
	ASP	T1446
	ASP	T1447
	ASP	T1448
	VAL	T1449
	GLU	T1450
	GLU	T1451

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79970	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 ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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	0.25	0/11752	0.48	0/15940

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	11511	0	11670	271	0
All	All	11511	0	11670	271	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 12.

The worst 5 of 271 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:767:GLN:NE2	1:A:786:ASP:O	2.12	0.83
1:A:518:GLU:HG2	1:A:519:PRO:HD3	1.60	0.83
1:A:894:ILE:HG13	1:A:1254:TRP:HE3	1.44	0.80
1:A:1149:ARG:HE	1:A:1264:THR:HG21	1.48	0.79
1:A:1447:LEU:HD21	1:A:1478:THR:HG21	1.68	0.76

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	1451/1565 (93%)	1415 (98%)	35 (2%)	1 (0%)	48 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	ASP

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	1274/1392 (92%)	1269 (100%)	5 (0%)	89 91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	493	LYS
1	A	1063	ASN
1	A	1079	ARG
1	A	1442	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1057	HIS

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.