



## wwPDB EM Validation Summary Report ⓘ

Oct 15, 2024 – 12:07 PM JST

PDB ID : 8IZ7  
EMDB ID : EMD-35834  
Title : cryo-EM structure of sulindac-bound hMRP4  
Authors : Liu, Z.M.; Huang, Y.  
Deposited on : 2023-04-06  
Resolution : 3.80 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](mailto: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>.

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

EMDB validation analysis	: <b>FAILED</b>
Mogul	: 1.8.5 (274361), CSD as541be (2020)
MolProbity	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: <b>FAILED</b>
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.39

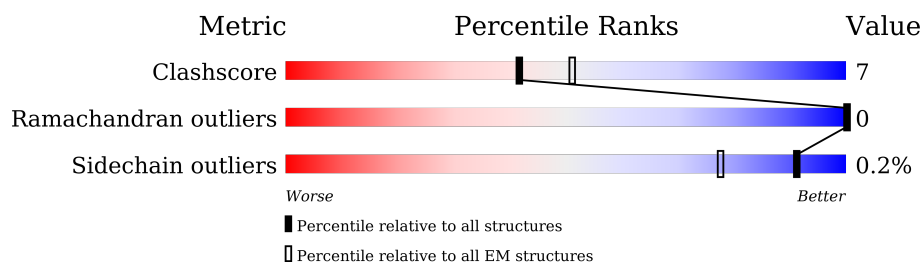
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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  $\geq 3$ , 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SUZ	A	1401	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9846 atoms, of which 16 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
			Total	C	N	O	S		
1	A	1229	9805	6365	1650	1747	43	0	0

There are 32 discrepancies between the modelled and reference sequences:

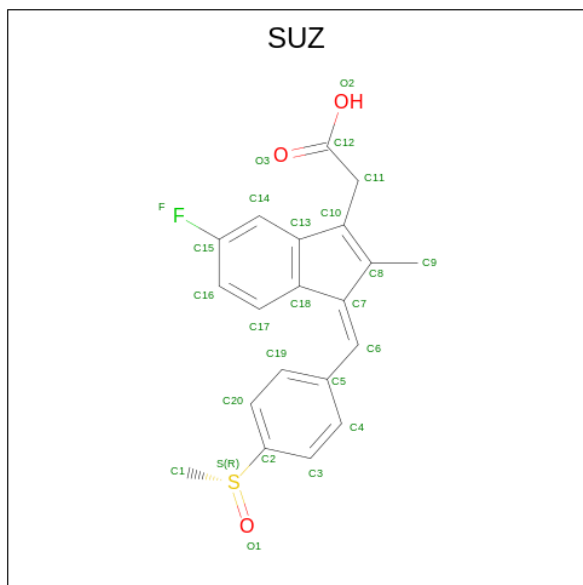
Chain	Residue	Modelled	Actual	Comment	Reference
A	1326	LEU	-	expression tag	UNP O15439
A	1327	GLU	-	expression tag	UNP O15439
A	1328	GLY	-	expression tag	UNP O15439
A	1329	GLY	-	expression tag	UNP O15439
A	1330	GLY	-	expression tag	UNP O15439
A	1331	SER	-	expression tag	UNP O15439
A	1332	GLY	-	expression 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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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

- Molecule 2 is [(1Z)-5-fluoro-2-methyl-1-{4-[methylsulfinyl]benzylidene}-1H-inden-3-yl]acetic acid (three-letter code: SUZ) (formula: C<sub>20</sub>H<sub>17</sub>FO<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).

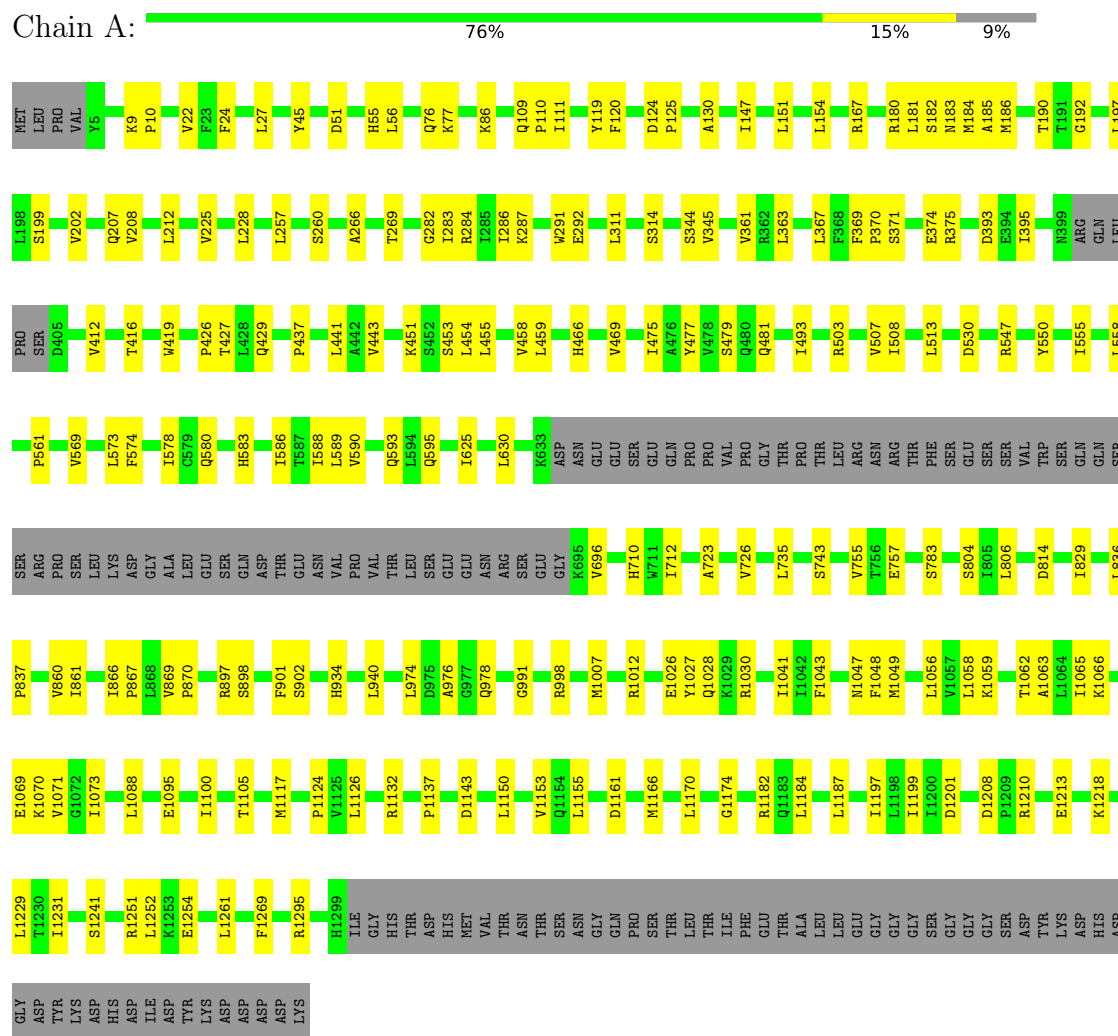


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	F	H	O	S	0
			41	20	1	16	3	1	

### 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 4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151694	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	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SUZ

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	0.24	0/10015	0.39	1/13571 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	197	LEU	CA-CB-CG	5.27	127.42	115.30

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	9805	0	10060	126	0
2	A	25	16	16	10	0
All	All	9830	16	10076	131	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 7.

The worst 5 of 131 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:998:ARG:NH1	2:A:1401:SUZ:O3	2.22	0.72
1:A:1041:ILE:HG23	1:A:1100:ILE:HG22	1.77	0.66
1:A:190:THR:HG22	1:A:192:GLY:H	1.61	0.64
1:A:51:ASP:HB2	1:A:56:LEU:HG	1.82	0.61
1:A:426:PRO:HG2	1:A:429:GLN:HG2	1.83	0.61

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	1223/1357 (90%)	1159 (95%)	64 (5%)	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	1070/1184 (90%)	1068 (100%)	2 (0%)	92	94

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

Mol	Chain	Res	Type
1	A	184	MET
1	A	1012	ARG



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	903	HIS
1	A	934	HIS
1	A	122	ASN
1	A	55	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SUZ	A	1401	-	27,27,27	3.11	9 (33%)	35,39,39	2.04	9 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SUZ	A	1401	-	-	7/12/28/28	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	SUZ	C6-C7	9.66	1.49	1.34
2	A	1401	SUZ	C2-S	-6.47	1.56	1.78
2	A	1401	SUZ	C10-C8	5.85	1.49	1.36
2	A	1401	SUZ	O1-S	5.13	1.63	1.49
2	A	1401	SUZ	C13-C18	3.97	1.47	1.39

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	SUZ	C17-C18-C13	-6.13	114.18	121.07
2	A	1401	SUZ	C1-S-C2	4.50	110.90	97.95
2	A	1401	SUZ	C17-C18-C7	3.94	140.94	133.78
2	A	1401	SUZ	C12-C11-C10	-3.33	104.39	113.71
2	A	1401	SUZ	F-C15-C14	3.26	122.91	118.25

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	SUZ	C13-C10-C11-C12
2	A	1401	SUZ	C20-C2-S-O1
2	A	1401	SUZ	C20-C2-S-C1
2	A	1401	SUZ	C3-C2-S-O1
2	A	1401	SUZ	C3-C2-S-C1

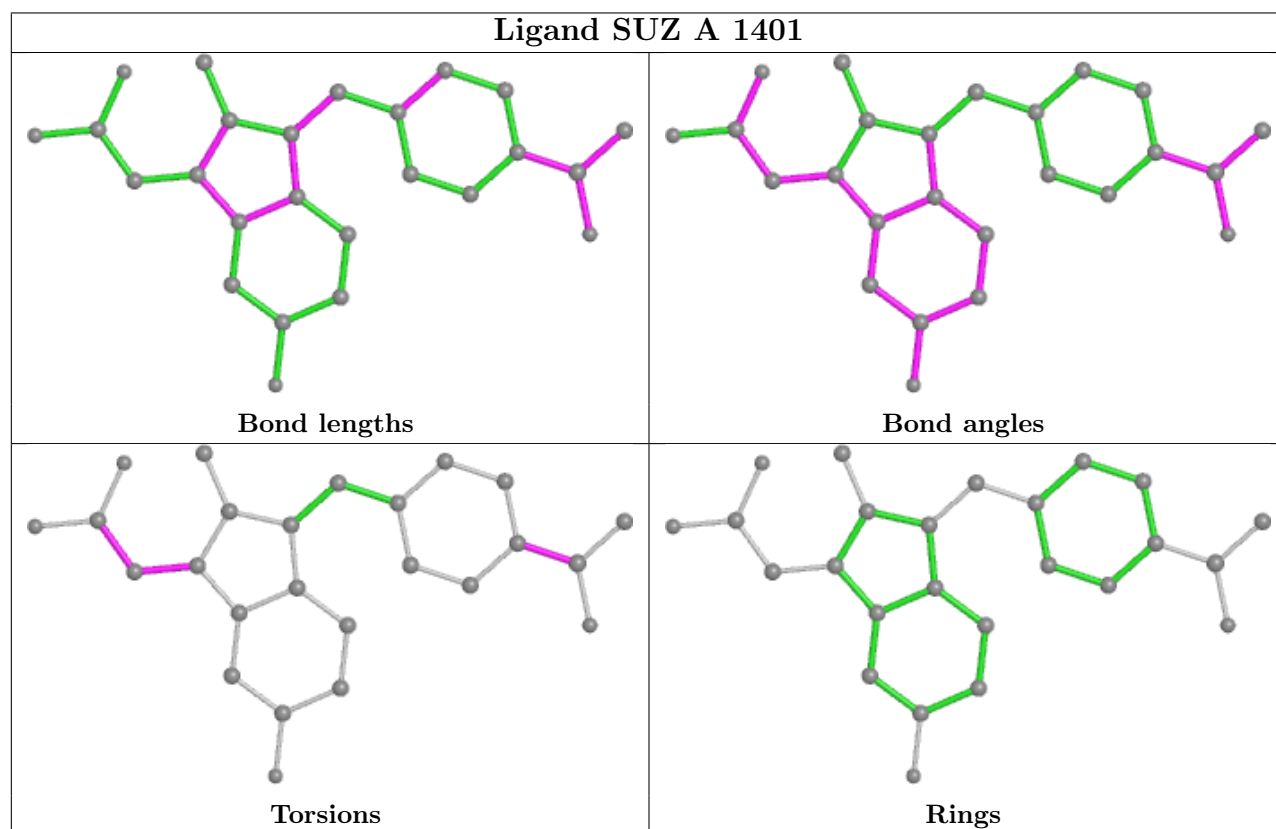
There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	SUZ	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.