



## wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 02:11 PM JST

PDB ID : 8J23  
EMDB ID : EMD-35943  
Title : Cryo-EM structure of FFAR2 complex in apo state  
Authors : Tai, L.; Li, F.; Sun, X.; Tang, W.; Wang, J.  
Deposited on : 2023-04-14  
Resolution : 3.20 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 : **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

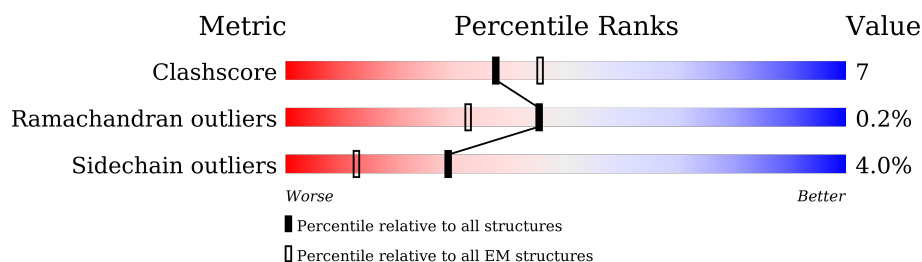
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	311	
2	B	354	
3	C	377	
4	D	71	
5	F	297	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8596 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 Free fatty acid receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	258	Total	C	N	O	S	0	0
			2084	1405	338	330	11		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	THR	LEU	conflict	UNP O15552
A	36	VAL	ILE	conflict	UNP O15552
A	80	ILE	VAL	variant	UNP O15552
A	86	GLY	SER	conflict	UNP O15552
A	148J	ASN	SER	variant	UNP O15552
A	170	GLU	ASN	conflict	UNP O15552
A	207	THR	SER	conflict	UNP O15552
A	210	HIS	LEU	variant	UNP O15552
A	245	PHE	TYR	variant	UNP O15552
A	246	TYR	HIS	conflict	UNP O15552
A	289	LEU	VAL	conflict	UNP O15552

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	216	Total	C	N	O	S	0	0
			1698	1084	284	318	12		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	340	Total	C	N	O	S	0	0
			2610	1609	469	511	21		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	MET	-	initiating methionine	UNP P62873
C	-11	HIS	-	expression tag	UNP P62873
C	-10	HIS	-	expression tag	UNP P62873
C	-9	HIS	-	expression tag	UNP P62873
C	-8	HIS	-	expression tag	UNP P62873
C	-7	HIS	-	expression tag	UNP P62873
C	-6	HIS	-	expression tag	UNP P62873
C	-5	GLY	-	expression tag	UNP P62873
C	-4	SER	-	expression tag	UNP P62873
C	-3	LEU	-	expression tag	UNP P62873
C	-2	LEU	-	expression tag	UNP P62873
C	-1	GLN	-	expression tag	UNP P62873
C	339	GLY	-	expression tag	UNP P62873
C	340	SER	-	expression tag	UNP P62873
C	341	SER	-	expression tag	UNP P62873
C	342	GLY	-	expression tag	UNP P62873
C	343	GLY	-	expression tag	UNP P62873
C	344	GLY	-	expression tag	UNP P62873
C	345	GLY	-	expression tag	UNP P62873
C	346	SER	-	expression tag	UNP P62873
C	347	GLY	-	expression tag	UNP P62873
C	348	GLY	-	expression tag	UNP P62873
C	349	GLY	-	expression tag	UNP P62873
C	350	GLY	-	expression tag	UNP P62873
C	351	SER	-	expression tag	UNP P62873
C	352	SER	-	expression tag	UNP P62873
C	353	GLY	-	expression tag	UNP P62873
C	354	VAL	-	expression tag	UNP P62873
C	355	SER	-	expression tag	UNP P62873
C	356	GLY	-	expression tag	UNP P62873
C	357	TRP	-	expression tag	UNP P62873
C	358	ARG	-	expression tag	UNP P62873
C	359	LEU	-	expression tag	UNP P62873
C	360	PHE	-	expression tag	UNP P62873
C	361	LYS	-	expression tag	UNP P62873
C	362	LYS	-	expression tag	UNP P62873
C	363	ILE	-	expression tag	UNP P62873
C	364	SER	-	expression tag	UNP P62873

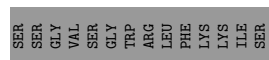
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	57	Total 433	C 271	N 75	O 84	S 3	0	0

- Molecule 5 is a protein called scFV16.

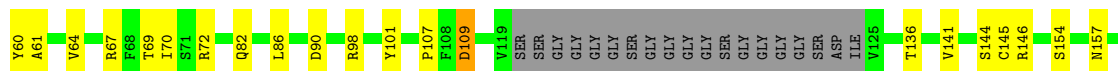
Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	230	Total 1771	C 1125	N 294	O 342	S 10	0	0





- |     |
|-----|
| MET |
| ALA |
| SER |
| ASN |
| N1  |
| E43 |
| D44 |
| P45 |
| L46 |
| L47 |
| F57 |
| ARG |
| GLU |
| LYS |
| LYS |
| PHE |
| PHE |
| CYS |
| ALA |
| ILE |
| LEU |

- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |    |    |    |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | LEU | VAL | ASN | GLN | SER | HIS | GLN | GLY | PHE | ASN | LYS | GLU | HIS | THR | SER | SER | LYS | MET | VAL | SER | ALA | ILE | VAL | LEU | TYR | VAL | LEU | LEU | ALA | ALA | ALA | HIS | SER | ALA | PHE | ALA | D1 | V2 | S7 | V12 | R18 | F29 | F32 | Q39 | A40 | K43 | G44 | L45 | S52 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	282601	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k 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	0.25	0/2147	0.47	0/2934
2	B	0.24	0/1727	0.44	0/2322
3	C	0.24	0/2657	0.51	1/3602 (0.0%)
4	D	0.23	0/439	0.41	0/594
5	F	0.25	0/1815	0.55	2/2460 (0.1%)
All	All	0.24	0/8785	0.49	3/11912 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	F	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	221	TYR	N-CA-C	7.72	131.84	111.00
5	F	222	PRO	CB-CA-C	5.08	124.71	112.00
3	C	151	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	220	GLU	Peptide
5	F	221	TYR	Peptide

## 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	2084	0	2166	32	0
2	B	1698	0	1654	21	0
3	C	2610	0	2516	49	0
4	D	433	0	444	4	0
5	F	1771	0	1714	30	0
All	All	8596	0	8494	125	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 125 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)
3:C:28:LEU:HD13	3:C:259:LEU:HD13	1.78	0.66
3:C:338:ASN:HD22	4:D:57:PHE:HB2	1.62	0.65
1:A:44:VAL:HG11	2:B:351:CYS:HA	1.80	0.64
5:F:39:GLN:HB2	5:F:45:LEU:HD23	1.78	0.64
5:F:217:GLN:NE2	5:F:222:PRO:O	2.33	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	254/311 (82%)	237 (93%)	17 (7%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	210/354 (59%)	209 (100%)	1 (0%)	0	100	100
3	C	338/377 (90%)	327 (97%)	11 (3%)	0	100	100
4	D	55/71 (78%)	55 (100%)	0	0	100	100
5	F	226/297 (76%)	217 (96%)	7 (3%)	2 (1%)	14	49
All	All	1083/1410 (77%)	1045 (96%)	36 (3%)	2 (0%)	45	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	221	TYR
5	F	222	PRO

### 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	226/270 (84%)	217 (96%)	9 (4%)	27	59
2	B	180/305 (59%)	175 (97%)	5 (3%)	38	68
3	C	282/308 (92%)	268 (95%)	14 (5%)	20	54
4	D	46/58 (79%)	45 (98%)	1 (2%)	47	73
5	F	194/239 (81%)	186 (96%)	8 (4%)	26	59
All	All	928/1180 (79%)	891 (96%)	37 (4%)	29	59

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	43	GLU
5	F	177	ARG
5	F	7	SER
5	F	144	SER
2	B	276	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
3	C	338	ASN

### 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.