



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 07:12 AM UTC

PDB ID : 4P4H / pdb_00004p4h
Title : Caught-in-action signaling complex of RIG-I 2CARD domain and MAVS CARD domain
Authors : Wu, B.; Hur, S.
Deposited on : 2014-03-12
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/XrayValidationReportHelp>

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:

MolProbity	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

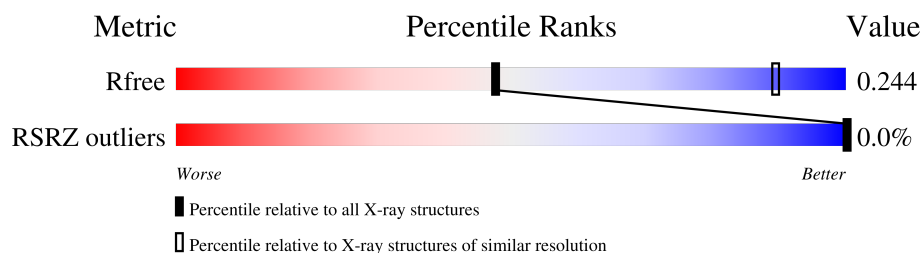
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 43332 atoms, of which 21621 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	188	Total	C	H	N	O	S	0	0	0
			3112	1007	1550	255	291	9			
1	B	189	Total	C	H	N	O	S	0	0	0
			3127	1012	1556	256	294	9			
1	C	189	Total	C	H	N	O	S	0	0	0
			3127	1012	1556	256	294	9			
1	D	188	Total	C	H	N	O	S	0	0	0
			3112	1007	1550	255	291	9			
1	E	188	Total	C	H	N	O	S	0	0	0
			3073	1000	1524	250	290	9			
1	F	189	Total	C	H	N	O	S	0	0	0
			3085	1004	1530	250	292	9			
1	G	189	Total	C	H	N	O	S	0	0	0
			3111	1008	1548	256	290	9			
1	H	188	Total	C	H	N	O	S	0	0	0
			3112	1007	1550	255	291	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP O95786
A	-2	PRO	-	expression tag	UNP O95786
A	-1	GLY	-	expression tag	UNP O95786
A	0	ALA	-	expression tag	UNP O95786
A	52	ALA	GLU	engineered mutation	UNP O95786
B	-3	GLY	-	expression tag	UNP O95786
B	-2	PRO	-	expression tag	UNP O95786
B	-1	GLY	-	expression tag	UNP O95786
B	0	ALA	-	expression tag	UNP O95786
B	52	ALA	GLU	engineered mutation	UNP O95786
C	-3	GLY	-	expression tag	UNP O95786
C	-2	PRO	-	expression tag	UNP O95786
C	-1	GLY	-	expression tag	UNP O95786

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP O95786
C	52	ALA	GLU	engineered mutation	UNP O95786
D	-3	GLY	-	expression tag	UNP O95786
D	-2	PRO	-	expression tag	UNP O95786
D	-1	GLY	-	expression tag	UNP O95786
D	0	ALA	-	expression tag	UNP O95786
D	52	ALA	GLU	engineered mutation	UNP O95786
E	-3	GLY	-	expression tag	UNP O95786
E	-2	PRO	-	expression tag	UNP O95786
E	-1	GLY	-	expression tag	UNP O95786
E	0	ALA	-	expression tag	UNP O95786
E	52	ALA	GLU	engineered mutation	UNP O95786
F	-3	GLY	-	expression tag	UNP O95786
F	-2	PRO	-	expression tag	UNP O95786
F	-1	GLY	-	expression tag	UNP O95786
F	0	ALA	-	expression tag	UNP O95786
F	52	ALA	GLU	engineered mutation	UNP O95786
G	-3	GLY	-	expression tag	UNP O95786
G	-2	PRO	-	expression tag	UNP O95786
G	-1	GLY	-	expression tag	UNP O95786
G	0	ALA	-	expression tag	UNP O95786
G	52	ALA	GLU	engineered mutation	UNP O95786
H	-3	GLY	-	expression tag	UNP O95786
H	-2	PRO	-	expression tag	UNP O95786
H	-1	GLY	-	expression tag	UNP O95786
H	0	ALA	-	expression tag	UNP O95786
H	52	ALA	GLU	engineered mutation	UNP O95786

- Molecule 2 is a protein called Mitochondrial antiviral-signaling protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	I	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	J	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	K	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	L	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	N	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	O	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	P	97	Total	C	H	N	O	S	0	0	0
			1586	511	790	139	140	6			
2	M	97	Total	C	H	N	O	S	0	0	0
			1581	511	785	139	140	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	GLY	-	expression tag	UNP Q7Z434
I	-7	SER	-	expression tag	UNP Q7Z434
I	-6	GLY	-	expression tag	UNP Q7Z434
I	-5	THR	-	expression tag	UNP Q7Z434
I	-4	GLY	-	expression tag	UNP Q7Z434
I	-3	SER	-	expression tag	UNP Q7Z434
I	-2	THR	-	expression tag	UNP Q7Z434
I	-1	GLY	-	expression tag	UNP Q7Z434
I	0	SER	-	expression tag	UNP Q7Z434
I	23	LYS	ASP	engineered mutation	UNP Q7Z434
I	26	LYS	GLU	engineered mutation	UNP Q7Z434
I	80	LYS	GLU	engineered mutation	UNP Q7Z434
J	-8	GLY	-	expression tag	UNP Q7Z434
J	-7	SER	-	expression tag	UNP Q7Z434
J	-6	GLY	-	expression tag	UNP Q7Z434
J	-5	THR	-	expression tag	UNP Q7Z434
J	-4	GLY	-	expression tag	UNP Q7Z434
J	-3	SER	-	expression tag	UNP Q7Z434
J	-2	THR	-	expression tag	UNP Q7Z434
J	-1	GLY	-	expression tag	UNP Q7Z434
J	0	SER	-	expression tag	UNP Q7Z434
J	23	LYS	ASP	engineered mutation	UNP Q7Z434
J	26	LYS	GLU	engineered mutation	UNP Q7Z434
J	80	LYS	GLU	engineered mutation	UNP Q7Z434
K	-8	GLY	-	expression tag	UNP Q7Z434
K	-7	SER	-	expression tag	UNP Q7Z434
K	-6	GLY	-	expression tag	UNP Q7Z434
K	-5	THR	-	expression tag	UNP Q7Z434
K	-4	GLY	-	expression tag	UNP Q7Z434
K	-3	SER	-	expression tag	UNP Q7Z434
K	-2	THR	-	expression tag	UNP Q7Z434
K	-1	GLY	-	expression tag	UNP Q7Z434
K	0	SER	-	expression tag	UNP Q7Z434
K	23	LYS	ASP	engineered mutation	UNP Q7Z434

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Chain	Residue	Modelled	Actual	Comment	Reference
K	26	LYS	GLU	engineered mutation	UNP Q7Z434
K	80	LYS	GLU	engineered mutation	UNP Q7Z434
L	-8	GLY	-	expression tag	UNP Q7Z434
L	-7	SER	-	expression tag	UNP Q7Z434
L	-6	GLY	-	expression tag	UNP Q7Z434
L	-5	THR	-	expression tag	UNP Q7Z434
L	-4	GLY	-	expression tag	UNP Q7Z434
L	-3	SER	-	expression tag	UNP Q7Z434
L	-2	THR	-	expression tag	UNP Q7Z434
L	-1	GLY	-	expression tag	UNP Q7Z434
L	0	SER	-	expression tag	UNP Q7Z434
L	23	LYS	ASP	engineered mutation	UNP Q7Z434
L	26	LYS	GLU	engineered mutation	UNP Q7Z434
L	80	LYS	GLU	engineered mutation	UNP Q7Z434
N	-8	GLY	-	expression tag	UNP Q7Z434
N	-7	SER	-	expression tag	UNP Q7Z434
N	-6	GLY	-	expression tag	UNP Q7Z434
N	-5	THR	-	expression tag	UNP Q7Z434
N	-4	GLY	-	expression tag	UNP Q7Z434
N	-3	SER	-	expression tag	UNP Q7Z434
N	-2	THR	-	expression tag	UNP Q7Z434
N	-1	GLY	-	expression tag	UNP Q7Z434
N	0	SER	-	expression tag	UNP Q7Z434
N	23	LYS	ASP	engineered mutation	UNP Q7Z434
N	26	LYS	GLU	engineered mutation	UNP Q7Z434
N	80	LYS	GLU	engineered mutation	UNP Q7Z434
O	-8	GLY	-	expression tag	UNP Q7Z434
O	-7	SER	-	expression tag	UNP Q7Z434
O	-6	GLY	-	expression tag	UNP Q7Z434
O	-5	THR	-	expression tag	UNP Q7Z434
O	-4	GLY	-	expression tag	UNP Q7Z434
O	-3	SER	-	expression tag	UNP Q7Z434
O	-2	THR	-	expression tag	UNP Q7Z434
O	-1	GLY	-	expression tag	UNP Q7Z434
O	0	SER	-	expression tag	UNP Q7Z434
O	23	LYS	ASP	engineered mutation	UNP Q7Z434
O	26	LYS	GLU	engineered mutation	UNP Q7Z434
O	80	LYS	GLU	engineered mutation	UNP Q7Z434
P	-8	GLY	-	expression tag	UNP Q7Z434
P	-7	SER	-	expression tag	UNP Q7Z434
P	-6	GLY	-	expression tag	UNP Q7Z434
P	-5	THR	-	expression tag	UNP Q7Z434

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-4	GLY	-	expression tag	UNP Q7Z434
P	-3	SER	-	expression tag	UNP Q7Z434
P	-2	THR	-	expression tag	UNP Q7Z434
P	-1	GLY	-	expression tag	UNP Q7Z434
P	0	SER	-	expression tag	UNP Q7Z434
P	23	LYS	ASP	engineered mutation	UNP Q7Z434
P	26	LYS	GLU	engineered mutation	UNP Q7Z434
P	80	LYS	GLU	engineered mutation	UNP Q7Z434
M	-8	GLY	-	expression tag	UNP Q7Z434
M	-7	SER	-	expression tag	UNP Q7Z434
M	-6	GLY	-	expression tag	UNP Q7Z434
M	-5	THR	-	expression tag	UNP Q7Z434
M	-4	GLY	-	expression tag	UNP Q7Z434
M	-3	SER	-	expression tag	UNP Q7Z434
M	-2	THR	-	expression tag	UNP Q7Z434
M	-1	GLY	-	expression tag	UNP Q7Z434
M	0	SER	-	expression tag	UNP Q7Z434
M	23	LYS	ASP	engineered mutation	UNP Q7Z434
M	26	LYS	GLU	engineered mutation	UNP Q7Z434
M	80	LYS	GLU	engineered mutation	UNP Q7Z434

- Molecule 3 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	S	71	Total	C	H	N	O	S	0	0	0
			1146	356	583	94	112	1			
3	T	73	Total	C	H	N	O	S	0	0	0
			1189	368	607	99	114	1			
3	U	72	Total	C	H	N	O	S	0	0	0
			1140	356	574	96	113	1			
3	W	71	Total	C	H	N	O	S	0	0	0
			1126	352	571	92	110	1			
3	X	73	Total	C	H	N	O	S	0	0	0
			1189	368	607	99	114	1			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	GLY	-	expression tag	UNP P62987
S	-1	PRO	-	expression tag	UNP P62987
S	0	GLY	-	expression tag	UNP P62987
T	-2	GLY	-	expression tag	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-1	PRO	-	expression tag	UNP P62987
T	0	GLY	-	expression tag	UNP P62987
U	-2	GLY	-	expression tag	UNP P62987
U	-1	PRO	-	expression tag	UNP P62987
U	0	GLY	-	expression tag	UNP P62987
W	-2	GLY	-	expression tag	UNP P62987
W	-1	PRO	-	expression tag	UNP P62987
W	0	GLY	-	expression tag	UNP P62987
X	-2	GLY	-	expression tag	UNP P62987
X	-1	PRO	-	expression tag	UNP P62987
X	0	GLY	-	expression tag	UNP P62987

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.81Å 117.33Å 257.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 3.40 46.80 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.80-3.40) 99.4 (46.80-3.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.191 , 0.240 0.203 , 0.244	Depositor DCC
R_{free} test set	2361 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	104.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 89.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	43332	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	188/205 (91%)	-0.65	0	100	100	61, 90, 138, 162	0
1	B	189/205 (92%)	-0.71	0	100	100	59, 92, 140, 174	0
1	C	189/205 (92%)	-0.74	0	100	100	58, 92, 163, 234	0
1	D	188/205 (91%)	-0.65	0	100	100	56, 83, 121, 161	0
1	E	188/205 (91%)	-0.57	0	100	100	75, 109, 145, 186	0
1	F	189/205 (92%)	-0.66	0	100	100	74, 112, 153, 179	0
1	G	189/205 (92%)	-0.64	0	100	100	60, 87, 130, 174	0
1	H	188/205 (91%)	-0.67	0	100	100	61, 94, 137, 183	0
2	I	97/108 (89%)	-0.57	0	100	100	52, 81, 131, 176	0
2	J	97/108 (89%)	-0.70	0	100	100	55, 80, 139, 156	0
2	K	97/108 (89%)	-0.77	0	100	100	56, 80, 112, 166	0
2	L	97/108 (89%)	-0.84	0	100	100	77, 110, 145, 165	0
2	M	97/108 (89%)	-0.46	0	100	100	108, 140, 195, 211	0
2	N	97/108 (89%)	-0.55	0	100	100	115, 155, 198, 210	0
2	O	97/108 (89%)	-0.45	0	100	100	110, 159, 207, 225	0
2	P	97/108 (89%)	-0.62	0	100	100	113, 158, 183, 220	0
3	S	71/79 (89%)	-0.69	0	100	100	77, 112, 149, 168	0
3	T	73/79 (92%)	-0.50	0	100	100	102, 147, 183, 196	1 (1%)
3	U	72/79 (91%)	-0.49	0	100	100	123, 189, 213, 225	0
3	W	71/79 (89%)	-0.66	1 (1%)	73	59	112, 157, 178, 206	0
3	X	73/79 (92%)	-0.67	0	100	100	82, 122, 152, 169	0
All	All	2644/2899 (91%)	-0.64	1 (0%)	100	100	52, 105, 180, 234	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	W	41	GLN	2.2

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.