



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 12, 2020 – 08:07 am GMT

PDB ID : 6TQR  
Title : The crystal structure of the MSP domain of human VAP-A in complex with the Phospho-FFAT motif of STARD3.  
Authors : McEwen, A.G.; Poussin-Courmontagne, P.; Di Mattia, T.; Wendling, C.; Cavarelli, J.; Tomasetto, C.; Alpy, F.  
Deposited on : 2019-12-17  
Resolution : 1.85 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.15.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.15.1

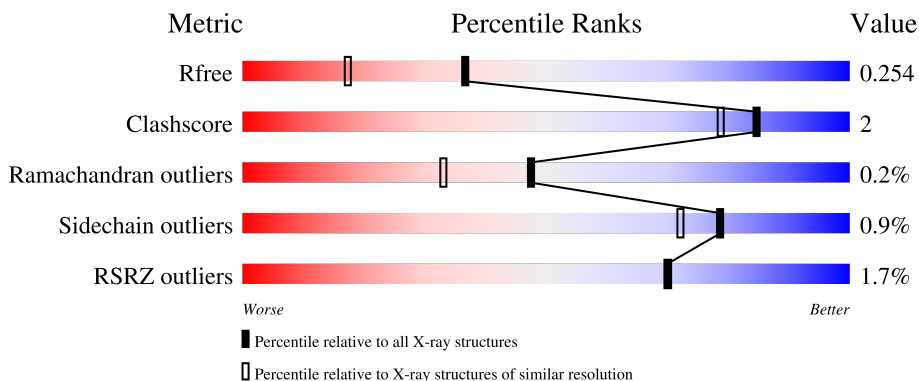
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	213	54% 41%
1	B	213	58% 41%
1	C	213	55% 41%
1	D	213	56% 41%
2	E	17	35% 29% 35%

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Mol	Chain	Length	Quality of chain
2	F	17	 <p>A horizontal bar chart showing the quality distribution of chain F. The bar is divided into five segments: a small red segment (6%), a green segment (18%), a yellow segment (18%), a small orange segment (6%), and a large grey segment (59%).</p>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4579 atoms, of which 0 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 Vesicle-associated membrane protein-associated protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	126	1036	669	170	188	9	0	8	0
1	B	126	1005	642	172	182	9	0	2	0
1	C	126	1075	688	185	194	8	0	10	0
1	D	126	1016	651	175	182	8	0	4	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ALA	-	expression tag	UNP Q9P0L0
A	214	LEU	-	expression tag	UNP Q9P0L0
A	215	GLU	-	expression tag	UNP Q9P0L0
A	216	HIS	-	expression tag	UNP Q9P0L0
A	217	HIS	-	expression tag	UNP Q9P0L0
A	218	HIS	-	expression tag	UNP Q9P0L0
A	219	HIS	-	expression tag	UNP Q9P0L0
A	220	HIS	-	expression tag	UNP Q9P0L0
B	213	ALA	-	expression tag	UNP Q9P0L0
B	214	LEU	-	expression tag	UNP Q9P0L0
B	215	GLU	-	expression tag	UNP Q9P0L0
B	216	HIS	-	expression tag	UNP Q9P0L0
B	217	HIS	-	expression tag	UNP Q9P0L0
B	218	HIS	-	expression tag	UNP Q9P0L0
B	219	HIS	-	expression tag	UNP Q9P0L0
B	220	HIS	-	expression tag	UNP Q9P0L0
C	213	ALA	-	expression tag	UNP Q9P0L0
C	214	LEU	-	expression tag	UNP Q9P0L0
C	215	GLU	-	expression tag	UNP Q9P0L0
C	216	HIS	-	expression tag	UNP Q9P0L0
C	217	HIS	-	expression tag	UNP Q9P0L0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	218	HIS	-	expression tag	UNP Q9P0L0
C	219	HIS	-	expression tag	UNP Q9P0L0
C	220	HIS	-	expression tag	UNP Q9P0L0
D	213	ALA	-	expression tag	UNP Q9P0L0
D	214	LEU	-	expression tag	UNP Q9P0L0
D	215	GLU	-	expression tag	UNP Q9P0L0
D	216	HIS	-	expression tag	UNP Q9P0L0
D	217	HIS	-	expression tag	UNP Q9P0L0
D	218	HIS	-	expression tag	UNP Q9P0L0
D	219	HIS	-	expression tag	UNP Q9P0L0
D	220	HIS	-	expression tag	UNP Q9P0L0

- Molecule 2 is a protein called StAR-related lipid transfer protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	11	Total 91	C 55	N 12	O 22	P 2	0	0	1
2	F	7	Total 60	C 38	N 8	O 13	P 1	0	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Cl 3	0	0
3	D	2	Total 2	Cl 2	0	0
3	C	2	Total 2	Cl 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total 78	O 78	0	2
4	B	59	Total 59	O 59	0	2
4	C	79	Total 79	O 79	0	2
4	D	64	Total 65	O 65	0	2

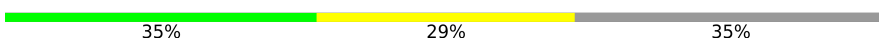
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	E	6	Total O 6 6	0	1
4	F	2	Total O 2 2	0	0




- Molecule 2: StAR-related lipid transfer protein 3

Chain E: 



- Molecule 2: StAR-related lipid transfer protein 3

Chain F: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.14Å 43.78Å 83.64Å 89.46° 92.91° 105.13°	Depositor
Resolution (Å)	42.26 – 1.85 83.53 – 1.85	Depositor EDS
% Data completeness (in resolution range)	53.7 (42.26-1.85) 53.7 (83.53-1.85)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 1.86Å)	Xtrriage
Refinement program	PHENIX dev-3699	Depositor
R, $R_{free}$	0.204 , 0.254 0.204 , 0.254	Depositor DCC
$R_{free}$ test set	1237 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 32.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 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: CL, SEP

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	0/1086	0.42	0/1474
1	B	0.25	0/1036	0.43	0/1406
1	C	0.25	0/1123	0.43	0/1520
1	D	0.25	0/1053	0.43	0/1429
2	E	0.29	0/73	0.38	0/95
2	F	0.24	0/52	0.38	0/68
All	All	0.25	0/4423	0.43	0/5992

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	1036	0	1057	7	0
1	B	1005	0	1014	2	0
1	C	1075	0	1103	4	0
1	D	1016	0	1033	4	0
2	E	91	0	65	3	0
2	F	60	0	46	3	0
3	A	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	1	0
3	D	2	0	0	0	0
4	A	78	0	0	2	0
4	B	59	0	0	0	0
4	C	79	0	0	0	0
4	D	65	0	0	0	0
4	E	6	0	0	0	0
4	F	2	0	0	0	0
All	All	4579	0	4318	20	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 2.

The worst 5 of 20 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:51[A]:VAL:HG12	1:A:97:VAL:HG22	1.80	0.63
1:D:52:LYS:NZ	2:F:209:SEP:OG	2.32	0.63
1:B:56:PRO:HB2	2:E:211:PRO:HG3	1.87	0.57
3:A:302:CL:CL	4:A:477:HOH:O	2.55	0.55
1:A:31:ASP:OD1	4:A:401:HOH:O	2.19	0.53

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 X-ray entries followed by that with respect to entries of similar resolution.

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	132/213 (62%)	131 (99%)	1 (1%)	0	100	100
1	B	126/213 (59%)	125 (99%)	1 (1%)	0	100	100
1	C	134/213 (63%)	131 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	128/213 (60%)	124 (97%)	2 (2%)	2 (2%)	9	2
2	E	7/17 (41%)	7 (100%)	0	0	100	100
2	F	4/17 (24%)	4 (100%)	0	0	100	100
All	All	531/886 (60%)	522 (98%)	7 (1%)	2 (0%)	47	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	10[A]	LYS
1	D	10[B]	LYS

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	122/198 (62%)	119 (98%)	3 (2%)	47	31
1	B	116/198 (59%)	116 (100%)	0	100	100
1	C	127/198 (64%)	125 (98%)	2 (2%)	62	49
1	D	117/198 (59%)	117 (100%)	0	100	100
2	E	7/9 (78%)	7 (100%)	0	100	100
2	F	5/9 (56%)	5 (100%)	0	100	100
All	All	494/810 (61%)	489 (99%)	5 (1%)	78	69

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

Mol	Chain	Res	Type
1	A	31	ASP
1	A	51[A]	VAL
1	A	51[B]	VAL
1	C	53	THR
1	C	134	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	98	GLN
2	E	206	GLN
2	F	206	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](#)

3 non-standard protein/DNA/RNA residues are 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	SEP	E	213	2	8,9,10	1.56	1 (12%)	8,12,14	1.62	2 (25%)
2	SEP	E	209	2	8,9,10	1.58	1 (12%)	8,12,14	1.26	1 (12%)
2	SEP	F	209	2	8,9,10	1.55	1 (12%)	8,12,14	1.32	1 (12%)

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	SEP	E	213	2	-	0/5/8/10	-
2	SEP	E	209	2	-	0/5/8/10	-
2	SEP	F	209	2	-	3/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	209	SEP	P-O1P	3.42	1.61	1.50
2	E	213	SEP	P-O1P	3.39	1.61	1.50
2	F	209	SEP	P-O1P	3.38	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	213	SEP	P-OG-CB	-3.12	109.69	118.30
2	E	213	SEP	OG-CB-CA	2.75	110.82	108.14
2	F	209	SEP	P-OG-CB	-2.59	111.17	118.30
2	E	209	SEP	P-OG-CB	-2.37	111.76	118.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	209	SEP	N-CA-CB-OG
2	F	209	SEP	CB-OG-P-O1P
2	F	209	SEP	CB-OG-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	209	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

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

### 6.1 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
1	A	126/213 (59%)	-0.21	2 (1%) 72 72	19, 31, 54, 88	0
1	B	126/213 (59%)	-0.09	2 (1%) 72 72	20, 32, 68, 117	0
1	C	126/213 (59%)	-0.10	2 (1%) 72 72	20, 32, 59, 84	0
1	D	126/213 (59%)	-0.15	2 (1%) 72 72	22, 34, 64, 76	0
2	E	9/17 (52%)	0.90	0 100 100	34, 52, 63, 68	0
2	F	6/17 (35%)	0.81	1 (16%) 1 1	36, 44, 72, 89	0
All	All	519/886 (58%)	-0.11	9 (1%) 70 70	19, 32, 64, 117	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ALA	6.3
1	C	95[A]	PHE	5.4
1	C	134	ASN	4.2
1	B	105	ASN	3.8
2	F	211	PRO	2.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SEP	E	209	10/11	0.90	0.13	51,58,61,62	0
2	SEP	E	213	10/11	0.91	0.15	60,61,62,63	0
2	SEP	F	209	10/11	0.91	0.14	53,59,65,66	0



### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	C	302	1/1	0.94	0.06	55,55,55,55	0
3	CL	A	301	1/1	0.96	0.07	47,47,47,47	0
3	CL	A	303	1/1	0.99	0.10	49,49,49,49	0
3	CL	D	302	1/1	0.99	0.07	38,38,38,38	0
3	CL	D	301	1/1	0.99	0.07	31,31,31,31	0
3	CL	A	302	1/1	0.99	0.07	53,53,53,53	0
3	CL	C	301	1/1	0.99	0.07	44,44,44,44	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.