



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:51 PM GMT

PDB ID : 3V99  
Title : S663D Stable-5-LOX in complex with Arachidonic Acid  
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Deposited on : 2011-12-23  
Resolution : 2.25 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

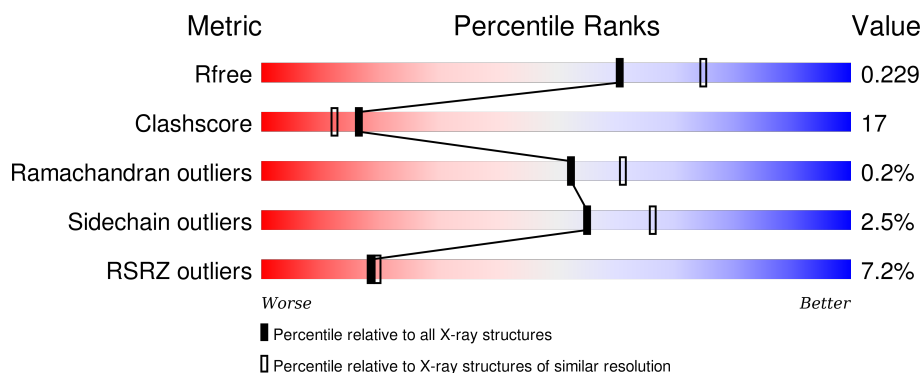
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	691	<div> <div>6%</div> <div>65%</div> <div>25%</div> <div>9%</div> </div>
1	B	691	<div> <div>8%</div> <div>71%</div> <div>20%</div> <div>8%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10799 atoms, of which 31 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 Arachidonate 5-lipoxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	2	0
			5147	3305	867	953	22			
1	B	639	Total	C	N	O	S	0	0	0
			5205	3336	889	958	22			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	EXPRESSION TAG	UNP P09917
A	-16	GLY	-	EXPRESSION TAG	UNP P09917
A	-15	SER	-	EXPRESSION TAG	UNP P09917
A	-14	SER	-	EXPRESSION TAG	UNP P09917
A	-13	HIS	-	EXPRESSION TAG	UNP P09917
A	-12	HIS	-	EXPRESSION TAG	UNP P09917
A	-11	HIS	-	EXPRESSION TAG	UNP P09917
A	-10	HIS	-	EXPRESSION TAG	UNP P09917
A	-9	HIS	-	EXPRESSION TAG	UNP P09917
A	-8	HIS	-	EXPRESSION TAG	UNP P09917
A	-7	SER	-	EXPRESSION TAG	UNP P09917
A	-6	SER	-	EXPRESSION TAG	UNP P09917
A	-5	GLY	-	EXPRESSION TAG	UNP P09917
A	-4	LEU	-	EXPRESSION TAG	UNP P09917
A	-3	VAL	-	EXPRESSION TAG	UNP P09917
A	-2	PRO	-	EXPRESSION TAG	UNP P09917
A	-1	ARG	-	EXPRESSION TAG	UNP P09917
A	0	GLY	-	EXPRESSION TAG	UNP P09917
A	1	SER	-	EXPRESSION TAG	UNP P09917
A	2	HIS	-	EXPRESSION TAG	UNP P09917
A	16	GLU	TRP	ENGINEERED MUTATION	UNP P09917
A	17	HIS	PHE	ENGINEERED MUTATION	UNP P09917
A	43	GLY	ASN	SEE REMARK 999	UNP P09917
A	44	SER	ASP	SEE REMARK 999	UNP P09917
A	75	GLY	TRP	ENGINEERED MUTATION	UNP P09917

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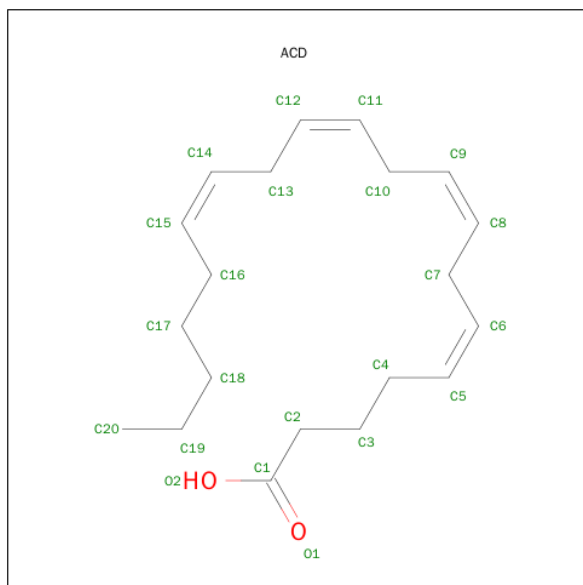
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Chain	Residue	Modelled	Actual	Comment	Reference
A	76	SER	LEU	ENGINEERED MUTATION	UNP P09917
A	240	ALA	CYS	ENGINEERED MUTATION	UNP P09917
A	561	ALA	CYS	ENGINEERED MUTATION	UNP P09917
A	653	GLU	LYS	ENGINEERED MUTATION	UNP P09917
A	654	ASN	LYS	ENGINEERED MUTATION	UNP P09917
A	655	LEU	LYS	ENGINEERED MUTATION	UNP P09917
A	663	ASP	SER	ENGINEERED MUTATION	UNP P09917
B	-12	MET	-	EXPRESSION TAG	UNP P09917
B	-11	GLY	-	EXPRESSION TAG	UNP P09917
B	-10	SER	-	EXPRESSION TAG	UNP P09917
B	-9	SER	-	EXPRESSION TAG	UNP P09917
B	-8	HIS	-	EXPRESSION TAG	UNP P09917
B	-7	HIS	-	EXPRESSION TAG	UNP P09917
B	-6	HIS	-	EXPRESSION TAG	UNP P09917
B	-5	HIS	-	EXPRESSION TAG	UNP P09917
B	-4	HIS	-	EXPRESSION TAG	UNP P09917
B	-3	HIS	-	EXPRESSION TAG	UNP P09917
B	-3A	SER	-	EXPRESSION TAG	UNP P09917
B	-3B	SER	-	EXPRESSION TAG	UNP P09917
B	-3C	GLY	-	EXPRESSION TAG	UNP P09917
B	-3D	LEU	-	EXPRESSION TAG	UNP P09917
B	-3E	VAL	-	EXPRESSION TAG	UNP P09917
B	-3F	PRO	-	EXPRESSION TAG	UNP P09917
B	-3G	ARG	-	EXPRESSION TAG	UNP P09917
B	-3H	GLY	-	EXPRESSION TAG	UNP P09917
B	-3I	SER	-	EXPRESSION TAG	UNP P09917
B	-3J	HIS	-	EXPRESSION TAG	UNP P09917
B	16	GLU	TRP	ENGINEERED MUTATION	UNP P09917
B	17	HIS	PHE	ENGINEERED MUTATION	UNP P09917
B	43	GLY	ASN	SEE REMARK 999	UNP P09917
B	44	SER	ASP	SEE REMARK 999	UNP P09917
B	75	GLY	TRP	ENGINEERED MUTATION	UNP P09917
B	76	SER	LEU	ENGINEERED MUTATION	UNP P09917
B	240	ALA	CYS	ENGINEERED MUTATION	UNP P09917
B	561	ALA	CYS	ENGINEERED MUTATION	UNP P09917
B	653	GLU	LYS	ENGINEERED MUTATION	UNP P09917
B	654	ASN	LYS	ENGINEERED MUTATION	UNP P09917
B	655	LEU	LYS	ENGINEERED MUTATION	UNP P09917
B	663	ASP	SER	ENGINEERED MUTATION	UNP P09917

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0

- Molecule 3 is ARACHIDONIC ACID (three-letter code: ACD) (formula:  $C_{20}H_{32}O_2$ ).

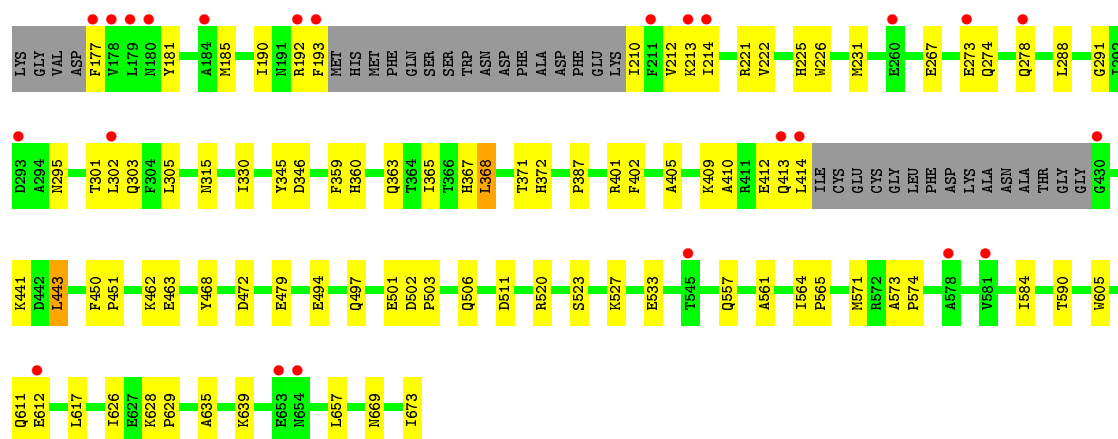


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 53 20 31 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	188	Total O 188 188	0	0
4	B	204	Total O 204 204	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.76 Å   200.84 Å   72.18 Å 90.00°   105.65°   90.00°	Depositor
Resolution (Å)	35.57 – 2.25 35.57 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.8 (35.57-2.25) 93.9 (35.57-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.30 (at 2.24 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.186   ,   0.233 0.186   ,   0.229	Depositor DCC
$R_{free}$ test set	2000 reflections (3.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 62626 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10799	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, ACD

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	0/5278	0.40	0/7160
1	B	0.23	0/5336	0.40	0/7240
All	All	0.23	0/10614	0.40	0/14400

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

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	5147	0	5035	192	0
1	B	5205	0	5101	149	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	31	31	5	0
4	A	188	0	0	18	0
4	B	204	0	0	12	0
All	All	10768	31	10167	340	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 17.

The worst 5 of 340 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:B:73:LYS:NZ	1:B:77:ASN:HA	1.45	1.32
1:A:367:HIS:O	1:A:371:THR:HG22	1.61	0.99
1:B:210:ILE:N	4:B:985:HOH:O	1.95	0.98
1:A:22:ASP:OD1	4:A:968:HOH:O	1.85	0.95
1:B:73:LYS:HZ1	1:B:77:ASN:HA	1.07	0.95

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	620/691 (90%)	605 (98%)	15 (2%)	0	100	100
1	B	629/691 (91%)	615 (98%)	11 (2%)	3 (0%)	34	34
All	All	1249/1382 (90%)	1220 (98%)	26 (2%)	3 (0%)	52	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	ASP
1	B	105	GLY
1	B	43	GLY

### 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	559/608 (92%)	544 (97%)	15 (3%)	52	63
1	B	565/608 (93%)	552 (98%)	13 (2%)	58	69
All	All	1124/1216 (92%)	1096 (98%)	28 (2%)	55	66

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	TYR
1	B	-6	HIS
1	B	443	LEU
1	A	511	ASP
1	A	610	PHE

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

Mol	Chain	Res	Type
1	B	295	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
3	ACD	A	702	-	18,21,21	0.59	0	18,21,21	0.89	1 (5%)

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
3	ACD	A	702	-	-	0/17/19/19	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	ACD	C2-C3-C4	2.87	118.90	113.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	ACD	5	0

## 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	630/691 (91%)	0.22	40 (6%) 23 25	13, 28, 65, 113	0
1	B	639/691 (92%)	0.32	52 (8%) 15 16	13, 28, 68, 118	0
All	All	1269/1382 (91%)	0.27	92 (7%) 18 20	13, 28, 65, 118	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	PHE	10.4
1	A	187	ASN	9.4
1	A	42	LYS	7.8
1	B	77	ASN	6.7
1	B	76	SER	6.3

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACD	A	702	22/22	0.51	0.31	1.11	50,71,90,98	0
2	FE2	B	701	1/1	0.99	0.13	-3.15	16,16,16,16	0
2	FE2	A	701	1/1	0.99	0.14	-	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.