



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 08:55 pm BST

PDB ID : 1CJY  
Title : HUMAN CYTOSOLIC PHOSPHOLIPASE A2  
Authors : Dessen, A.; Tang, J.; Schmidt, H.; Stahl, M.; Clark, J.D.; Seehra, J.; Somers, W.S.  
Deposited on : 1999-04-20  
Resolution : 2.50 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

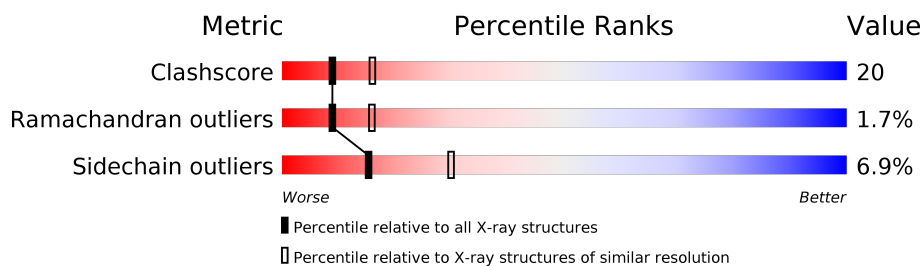
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	749	
1	B	749	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9706 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.

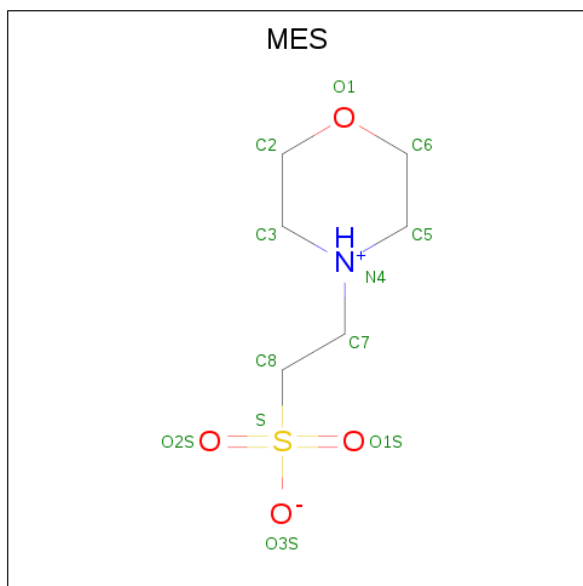
- Molecule 1 is a protein called PROTEIN (CYTOSOLIC PHOSPHOLIPASE A2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	0	0
			4876	3144	804	895	33			
1	B	614	Total	C	N	O	S	0	0	0
			4744	3066	773	871	34			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

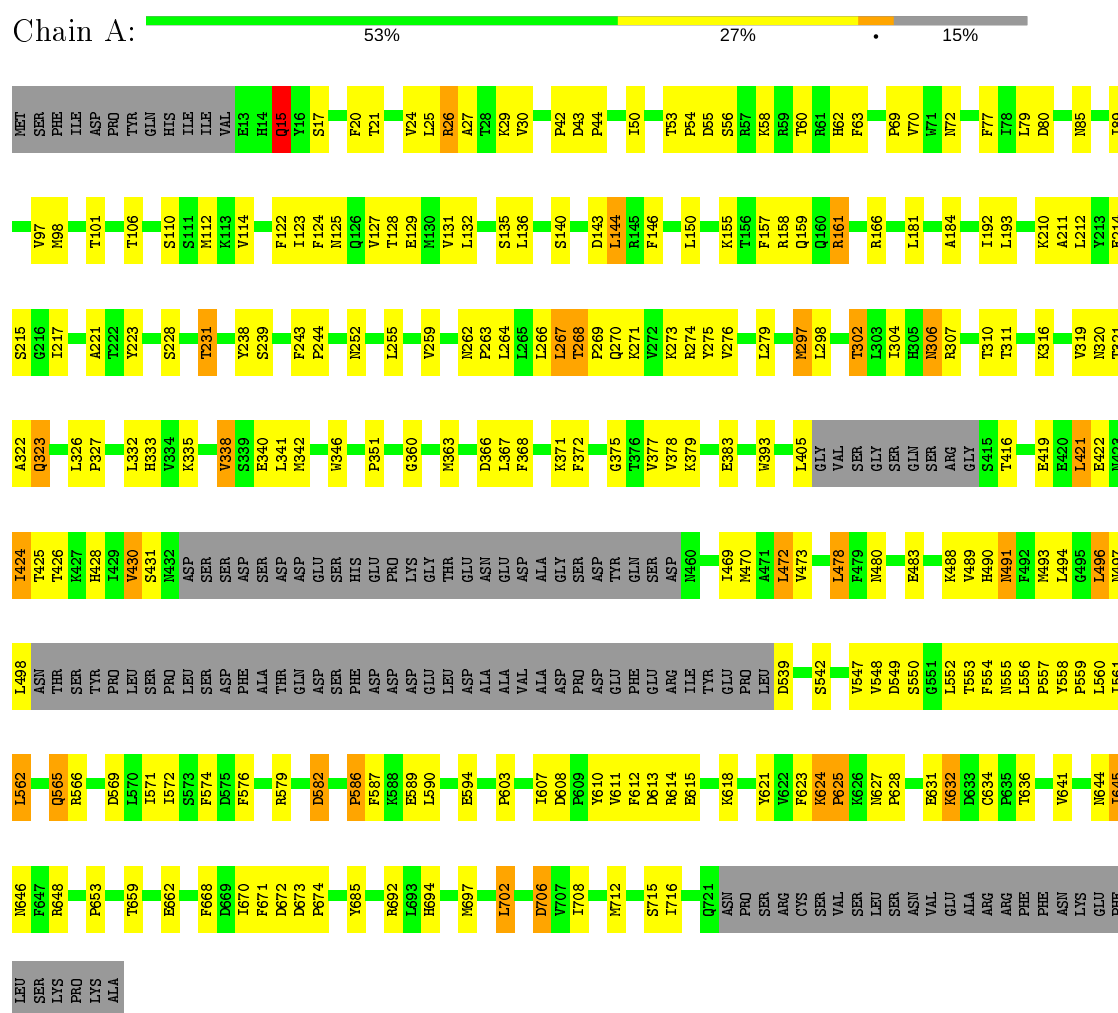
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	26	Total	O	0	0
			26	26		

### 3 Residue-property plots

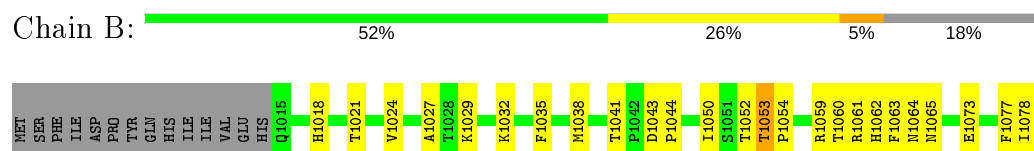
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: PROTEIN (CYTOSOLIC PHOSPHOLIPASE A2)



#### • Molecule 1: PROTEIN (CYTOSOLIC PHOSPHOLIPASE A2)



SER	V1641	LEU	S1476	SER	V1320	E1214	V1086
ASN	L1642	D1639	A1477	GLY	T1321	E1217	L1091
VAL	A1643	I1545	L1478	GLN	Q1323	D1219	V1097
GLU	M1644	H1546	F1479	SER	P1324	C1220	M1098
ALA	I1645	V1547	T1481	ARG	P1325		
ARG	M1646	V1548	R1482	GLY	F1329		T1101
ARG	Y1650	D1549	E1483		L1332		L1102
PHE	LYS	S1550	R1485	S1415	L1335		L1103
ASN	A1652	N1555	V1489	T1416	K1336		K1113
LYS		L1556	H1490	E1418	V1338		E1116
GLU	E1658	P1557	M1491	E1419	S1339		
PHE	T1659	Y1558	H1492	E1420	E1340		
LEU	E1660		M1493	L1421	I1341		I1123
SER	E1661	I1561	L1494		T1425		F1124
LYS	E1662	R1562		T1426	M1342		N1125
PRO		R1563		T1427	F1343		Q1126
LYS	I1670	P1564		H1428	F1349		V1127
ALA		Q1565	M1497	I1429	ASN		T1128
	E1675	R1566	LEU	V1430	Y1352		E1130
	S1676	G1567	THR	SER	M1363		V1131
	T1680	V1568	THR	ASN	A1364		L1132
			SER	ASP	P1365		
	Y1685	D1582	TVR	SER	D1366		S1135
	F1686	S1583	PRO	SER	P1367		D1143
	M1687	S1584	LEU	ASP	L1368		L1144
		P1585	PRO	SER	F1369		
	F1690	P1586	LEU	ASP	G1370		F1157
		L1590	LEU	ASP	K1371		R1158
	L1696	K1595	ASP	GLU	F1372		
	H1697		ALA	SER	F1373		R1161
	H1698	M1600	THR	GLN	M1374		
		L1601	GLN	ASP	G1375		I1165
	L1702	L1602	ASP	GLY	T1376		
			SER	THR	V1377		L1172
	I1705	D1608	PHE	GLU	Y1381		L1173
	D1706	V1611	ASP	ASN	E1382		G1174
	V1707	F1612	ASP	GLU	E1383		
	K1709		GLU	ASP	N1384		N1177
		G1616	LEU	ALA			S1178
	V1713	L1617	ASP	GLY	H1387		E1179
		R1618	ALA	SER			G1180
	I1716	E1619	ALA	ASP	W1393		L1181
	E1717		VAL	TYR	M1397		
	TVR	P1625	ALA	GLN	F1397		A1184
	ARG	LYS	ASP	SER	S1398		R1185
	ARG	ASN	PRO	ASP	I1399		D1186
	GLN	PRO	ASP	ASN	L1400		V1187
	ASN	ASP	GLU	GLN	F1401		P1188
	PRO	MET	PHE	ALA	N1402		V1189
	SER	GLU	ARG	S1463	R1403		V1190
	ARG	LYS	ILE	H1464	V1404		A1191
	CYS		TYR	I1465	L1406		T1192
	SER	D1633	GLU	H1466	G1406		L1193
	VAL		PRO		VAL		
	SER	T1636		M1470			K1210
	LEU						

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.59 Å 95.49 Å 139.13 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.3 (12.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.229 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

## 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: CA, MES

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	0.39	0/4999	0.63	0/6796
1	B	0.40	0/4862	0.64	1/6603 (0.0%)
All	All	0.39	0/9861	0.63	1/13399 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1227	LEU	CA-CB-CG	5.49	127.94	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	4876	0	4668	203	0
1	B	4744	0	4576	181	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	12	0	13	0	0
3	B	12	0	13	1	0
4	A	32	0	0	1	0
4	B	26	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9706	0	9270	384	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 20.

The worst 5 of 384 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:323:GLN:N	1:A:323:GLN:HE21	1.54	1.04
1:A:79:LEU:HD22	1:A:85:ASN:HD22	1.23	1.03
1:A:323:GLN:NE2	1:A:323:GLN:H	1.59	0.99
1:B:1323:GLN:HE21	1:B:1323:GLN:H	1.08	0.98
1:B:1465:ILE:HD12	1:B:1465:ILE:H	1.26	0.97

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	625/749 (83%)	565 (90%)	48 (8%)	12 (2%)	8	13
1	B	602/749 (80%)	553 (92%)	40 (7%)	9 (2%)	10	18
All	All	1227/1498 (82%)	1118 (91%)	88 (7%)	21 (2%)	9	16

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	430	VAL
1	A	625	PRO
1	A	632	LYS
1	B	1178	SER

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Mol	Chain	Res	Type
1	B	1584	SER

### 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	519/677 (77%)	487 (94%)	32 (6%)	18	35
1	B	511/677 (76%)	472 (92%)	39 (8%)	13	25
All	All	1030/1354 (76%)	959 (93%)	71 (7%)	15	30

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1053	THR
1	B	1227	LEU
1	B	1590	LEU
1	B	1059	ARG
1	B	1128	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	694	HIS
1	B	1082	ASN
1	B	1694	HIS
1	A	704	ASN
1	B	1018	HIS

### 5.3.3 RNA [i](#)

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	MES	A	3000	2	12,12,12	9.06	8 (66%)	14,16,16	2.68	6 (42%)
3	MES	B	4000	2	12,12,12	8.86	8 (66%)	14,16,16	2.61	6 (42%)

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	MES	A	3000	2	-	1/6/14/14	0/1/1/1
3	MES	B	4000	2	-	2/6/14/14	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3000	MES	C8-S	-24.05	1.43	1.77
3	B	4000	MES	C8-S	-23.50	1.44	1.77
3	A	3000	MES	O1S-S	11.83	1.80	1.45
3	B	4000	MES	O2S-S	11.60	1.79	1.45
3	A	3000	MES	O2S-S	11.40	1.78	1.45

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	3000	MES	O3S-S-C8	5.79	115.14	105.77
3	B	4000	MES	O3S-S-C8	5.43	114.55	105.77
3	A	3000	MES	O1S-S-C8	5.26	113.24	106.92
3	B	4000	MES	O1S-S-C8	5.06	113.01	106.92
3	B	4000	MES	O2S-S-C8	3.52	111.15	106.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3000	MES	N4-C7-C8-S
3	B	4000	MES	N4-C7-C8-S
3	B	4000	MES	C7-C8-S-O2S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4000	MES	1	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.