



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2018 – 10:45 AM EST

PDB ID : 1A1A  
Title : C-SRC (SH2 DOMAIN WITH C188A MUTATION) COMPLEXED WITH  
ACE-FORMYL PHOSPHOTYR-GLU-(N,N-DIPENTYL AMINE)  
Authors : Shewchuk, L.; Jordan, S.  
Deposited on : 1997-12-10  
Resolution : 2.00 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

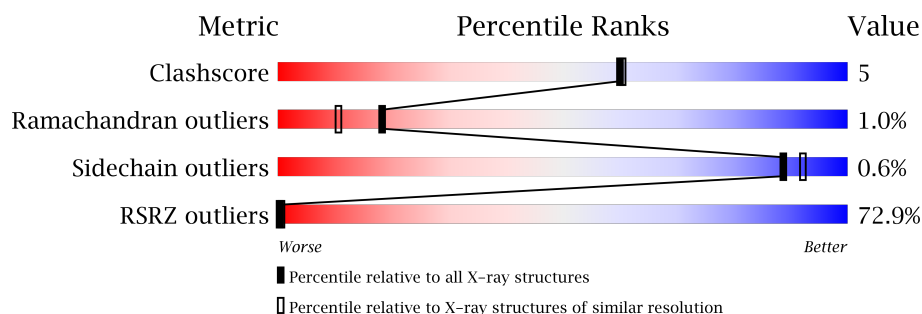
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	107	<div> <div>68%</div> <div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	107	<div> <div>74%</div> <div> <div>78%</div> <div>15%</div> <div>5%</div> </div> </div>
2	C	4	<div> <div>75%</div> <div>25%</div> </div>
2	D	4	<div> <div>25%</div> <div> <div>75%</div> <div>25%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2734 atoms, of which 800 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 C-SRC TYROSINE KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	106	Total	C	H	N	O	S	0	0	0
			1048	530	205	150	161	2			
1	B	102	Total	C	H	N	O	S	0	0	0
			1016	514	201	146	153	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	SER	CYS	ENGINEERED	UNP P12931
B	188	SER	CYS	ENGINEERED	UNP P12931

- Molecule 2 is a protein called ACE-FORMYL PHOSPHOTYR-GLU-(N,N-DIPENTYL AMINE).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	N	O	P	0	0	0
			44	27	3	3	10	1			
2	D	4	Total	C	H	N	O	P	0	0	0
			44	27	3	3	10	1			

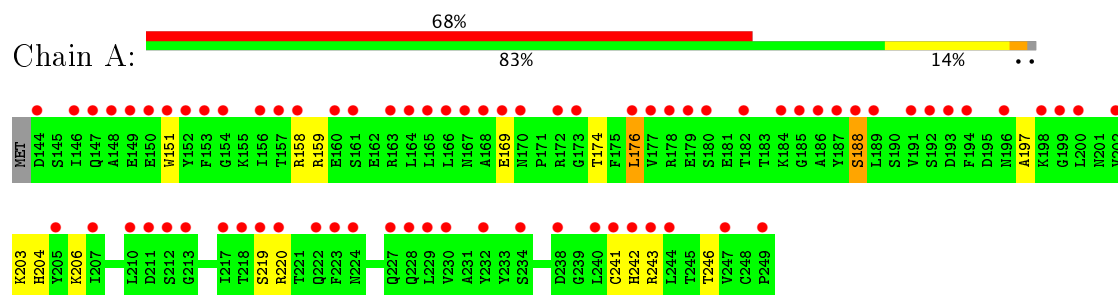
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	113	Total	H	O	0	0
			339	226	113		
3	C	3	Total	H	O	0	0
			9	6	3		
3	B	76	Total	H	O	0	0
			228	152	76		
3	D	2	Total	H	O	0	0
			6	4	2		

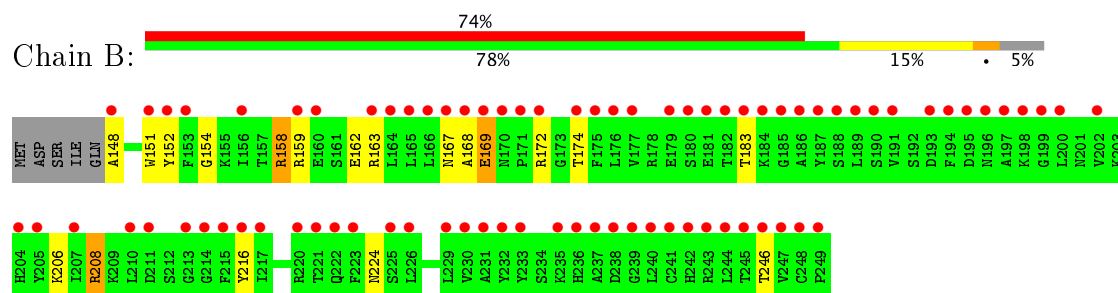
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

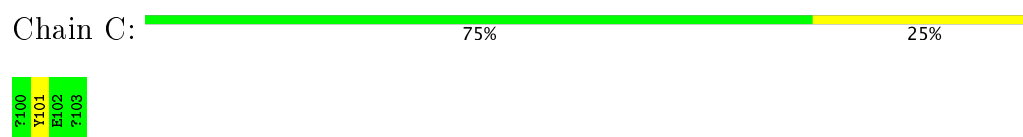
#### • Molecule 1: C-SRC TYROSINE KINASE



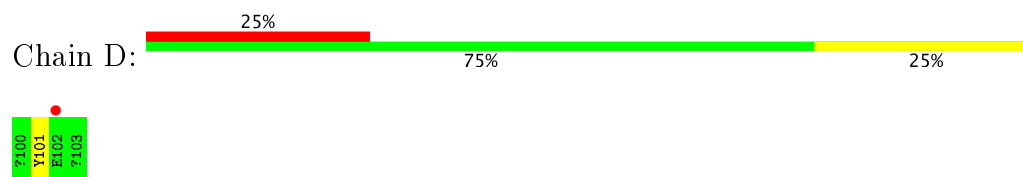
#### • Molecule 1: C-SRC TYROSINE KINASE



#### • Molecule 2: ACE-FORMYL PHOSPHOTYR-GLU-(N,N-DIPENTYL AMINE)



#### • Molecule 2: ACE-FORMYL PHOSPHOTYR-GLU-(N,N-DIPENTYL AMINE)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.40Å 65.40Å 74.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00 49.18 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (6.00-2.00) 90.1 (49.18-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 1.91Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.198 , (Not available) 0.448 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 69.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.74	EDS
Total number of atoms	2734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.54% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DIP, ACE, PTH

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	0.95	1/860 (0.1%)	1.30	7/1160 (0.6%)
1	B	0.98	1/832 (0.1%)	1.29	8/1121 (0.7%)
2	C	1.04	0/8	0.91	0/9
2	D	1.28	0/8	0.68	0/9
All	All	0.97	2/1708 (0.1%)	1.29	15/2299 (0.7%)

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
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	SER	CB-OG	6.20	1.50	1.42
1	B	169	GLU	C-N	5.10	1.45	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	TRP	CD1-CG-CD2	9.78	114.12	106.30
1	B	158	ARG	NE-CZ-NH2	-9.73	115.44	120.30
1	A	158	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	158	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	151	TRP	CD1-CG-CD2	8.30	112.94	106.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	LEU	Mainchain
1	B	169	GLU	Mainchain

## 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	843	205	810	9	3
1	B	815	201	792	8	11
2	C	41	3	38	1	0
2	D	41	3	39	1	0
3	A	113	226	0	2	10
3	B	76	152	0	2	2
3	C	3	6	0	0	0
3	D	2	4	0	0	0
All	All	1934	800	1679	18	13

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 5.

The worst 5 of 18 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:163:ARG:O	1:B:167:ASN:HB2	1.86	0.74
1:A:242:HIS:HD2	1:A:243:ARG:O	1.80	0.65
1:A:204:HIS:HB3	2:C:101:PTH:OF	1.97	0.64
1:A:174:THR:HA	1:A:246:THR:O	2.02	0.58
1:B:163:ARG:HG3	3:B:675:HOH:O	2.04	0.58

The worst 5 of 13 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ASN:HD22	3:A:529:HOH:O[4_456]	0.67	0.93
1:B:224:ASN:ND2	3:A:529:HOH:O[4_456]	1.40	0.80
1:B:159:ARG:HH12	3:A:503:HOH:H1[3_745]	0.91	0.69
1:A:169:GLU:O	1:B:172:ARG:HH22[4_456]	0.97	0.63
3:A:665:HOH:O	3:B:589:HOH:O[3_755]	1.65	0.55

## 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	104/107 (97%)	102 (98%)	1 (1%)	1 (1%)	18	10
1	B	100/107 (94%)	96 (96%)	3 (3%)	1 (1%)	18	10
2	C	1/4 (25%)	1 (100%)	0	0	100	100
2	D	1/4 (25%)	1 (100%)	0	0	100	100
All	All	206/222 (93%)	200 (97%)	4 (2%)	2 (1%)	18	10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	ALA
1	A	197	ALA

### 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	89/94 (95%)	88 (99%)	1 (1%)	78	82
1	B	86/94 (92%)	86 (100%)	0	100	100
2	C	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
All	All	177/190 (93%)	176 (99%)	1 (1%)	89	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	SER

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

Mol	Chain	Res	Type
1	A	222	GLN
1	A	242	HIS
1	B	170	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	PTH	C	101	2	17,18,19	1.38	3 (17%)	21,25,27	1.84	5 (23%)
2	PTH	D	101	2	17,18,19	1.79	3 (17%)	21,25,27	1.73	6 (28%)

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	PTH	C	101	2	-	0/11/13/15	0/1/1/1
2	PTH	D	101	2	-	0/11/13/15	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	101	PTH	CF-CE1	-4.82	1.38	1.51
2	D	101	PTH	OF-CF	-3.78	1.25	1.41
2	C	101	PTH	P-O1P	-2.72	1.41	1.50
2	C	101	PTH	OH-CZ	-2.46	1.36	1.40
2	D	101	PTH	P-O1P	-2.24	1.43	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	101	PTH	CD1-CE1-CZ	-4.13	113.80	118.30
2	D	101	PTH	O3P-P-OH	-3.91	91.69	105.63
2	D	101	PTH	CB-CA-C	-3.02	105.59	111.41
2	D	101	PTH	CF-CE1-CZ	-2.34	114.74	119.25
2	C	101	PTH	O3P-P-OH	-2.18	97.85	105.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	101	PTH	1	0
2	D	101	PTH	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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.

## 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	106/107 (99%)	2.53	73 (68%) 0 1	21, 33, 61, 72	0
1	B	102/107 (95%)	3.41	79 (77%) 0 0	22, 31, 66, 70	0
2	C	1/4 (25%)	0.88	0 100 100	34, 34, 34, 34	0
2	D	1/4 (25%)	2.27	1 (100%) 0 0	33, 33, 33, 33	0
All	All	210/222 (94%)	2.95	153 (72%) 0 0	21, 32, 64, 72	0

The worst 5 of 153 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	ALA	9.2
1	B	182	THR	8.2
1	B	167	ASN	7.6
1	B	223	PHE	6.7
1	B	200	LEU	6.6

### 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. 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(Å <sup>2</sup> )	Q<0.9
2	PTH	C	101	18/19	0.72	0.29	-	0,35,44,59	0
2	PTH	D	101	18/19	0.70	0.27	-	0,41,47,55	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.