



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 06:08 pm GMT

PDB ID : 1A08
Title : C-SRC (SH2 DOMAIN) COMPLEXED WITH ACE-DIFLUORO PHOSPH
OTYR-GLU-(N,N-DIPENTYL AMINE)
Authors : Shewchuk, L.; Jordan, S.
Deposited on : 1997-12-09
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

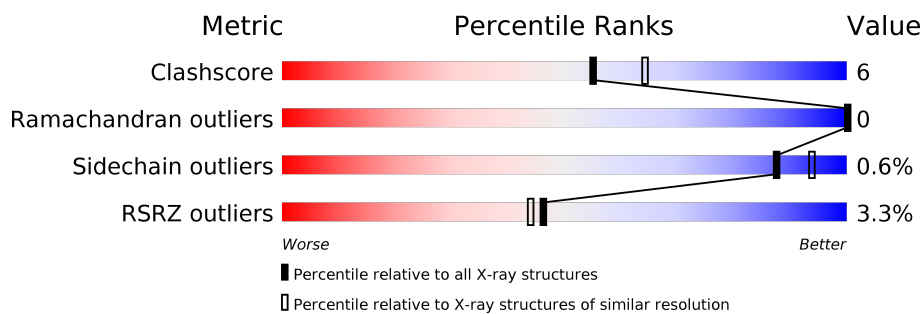
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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 ≥ 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>6%</div> <div>73% 21% . .</div> </div>
1	B	107	<div> <div>6%</div> <div>75% 19% . .</div> </div>
2	C	4	<div> <div>100%</div> </div>
2	D	4	<div> <div>75% 25%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2199 atoms, of which 448 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	105	Total	C	H	N	O	S	0	0	0
			1020	520	196	145	156	3			
1	B	104	Total	C	H	N	O	S	0	0	0
			1012	517	194	144	154	3			

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

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	C	4	Total	C	F	H	N	O	P	0	0	0
			43	27	2	2	3	8	1			
2	D	4	Total	C	F	H	N	O	P	0	0	0
			43	27	2	2	3	8	1			

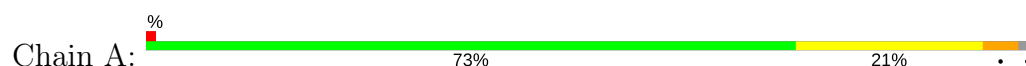
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	16	Total	H	O	0	0
			48	32	16		
3	C	3	Total	H	O	0	0
			9	6	3		
3	B	7	Total	H	O	0	0
			21	14	7		
3	D	1	Total	H	O	0	0
			3	2	1		

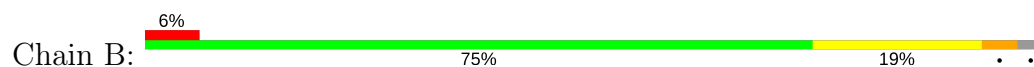
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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-DIFLUORO PHOSPHOTYR-GLU-(N,N-DIPENTYL AMINE)



There are no outlier residues recorded for this chain.

- Molecule 2: ACE-DIFLUORO 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, α , β , γ	51.90Å 67.40Å 75.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20 36.08 – 2.20	Depositor EDS
% Data completeness (in resolution range)	83.0 (6.00-2.20) 83.1 (36.08-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.192 , (Not available) 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 85.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2199	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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.

5 Model quality

5.1 Standard geometry

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

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	1.05	0/841	1.77	17/1136 (1.5%)
1	B	1.04	1/835 (0.1%)	1.79	19/1128 (1.7%)
2	C	1.23	0/8	0.93	0/9
2	D	1.43	0/8	0.87	0/9
All	All	1.05	1/1692 (0.1%)	1.77	36/2282 (1.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	240	LEU	C-N	-7.29	1.17	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ARG	NE-CZ-NH2	-12.71	113.95	120.30
1	A	158	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	B	220	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	A	158	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	A	216	TYR	CB-CG-CD1	-8.96	115.63	121.00
1	A	230	VAL	CG1-CB-CG2	-8.67	97.03	110.90
1	B	208	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	B	151	TRP	CE2-CD2-CG	-8.25	100.70	107.30
1	B	151	TRP	CG-CD2-CE3	8.09	141.18	133.90
1	A	216	TYR	CB-CG-CD2	8.04	125.82	121.00
1	A	232	TYR	CB-CG-CD2	-7.91	116.25	121.00
1	B	166	LEU	CA-C-N	-7.86	99.92	117.20
1	B	163	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	B	151	TRP	CB-CG-CD1	-7.54	117.20	127.00
1	B	208	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	A	182	THR	N-CA-CB	-7.27	96.48	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	B	222	GLN	CA-CB-CG	6.74	128.24	113.40
1	A	149	GLU	C-N-CA	6.46	137.84	121.70
1	B	209	LYS	CA-CB-CG	-6.32	99.49	113.40
1	A	163	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	158	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	158	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	159	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	167	ASN	CA-CB-CG	-5.96	100.29	113.40
1	A	243	ARG	CA-CB-CG	5.96	126.50	113.40
1	A	178	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	220	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	205	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	B	243	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	B	200	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	B	208	ARG	CB-CG-CD	5.25	125.26	111.60
1	A	158	ARG	CG-CD-NE	-5.24	100.79	111.80
1	B	240	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	B	220	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	177	VAL	CA-CB-CG2	-5.05	103.32	110.90

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	824	196	787	11	0
1	B	818	194	782	9	0
2	C	41	2	38	0	0
2	D	41	2	38	1	0
3	A	16	32	0	0	0
3	B	7	14	0	0	0
3	C	3	6	0	0	0
3	D	1	2	0	0	0
All	All	1751	448	1645	19	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 6.

All (19) 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:242:HIS:HD2	1:B:243:ARG:O	1.84	0.61
1:A:243:ARG:NH2	1:A:245:THR:HG22	2.15	0.60
1:B:188:CYS:SG	2:D:101:FTY:HE2	2.41	0.59
1:A:187:TYR:HB2	1:A:207:ILE:HB	1.83	0.59
1:B:220:ARG:NH1	1:B:238:ASP:OD2	2.36	0.59
1:A:146:ILE:HD11	1:A:151:TRP:CH2	2.38	0.58
1:A:146:ILE:HD12	1:A:149:GLU:HG3	1.86	0.58
1:B:174:THR:HA	1:B:246:THR:O	2.08	0.53
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.73	0.53
1:A:242:HIS:HD2	1:A:243:ARG:O	1.94	0.51
1:B:175:PHE:CD1	1:B:244:LEU:HB3	2.50	0.46
1:B:193:ASP:OD2	1:B:203:LYS:NZ	2.49	0.46
1:B:158:ARG:O	1:B:162:GLU:HG3	2.16	0.46
1:A:159:ARG:HH11	1:B:249:PRO:HA	1.81	0.45
1:A:174:THR:HA	1:A:246:THR:O	2.17	0.44
1:A:247:VAL:HG12	1:A:248:CYS:O	2.19	0.43
1:A:170:ASN:CG	1:A:174:THR:HG21	2.39	0.42
1:A:233:TYR:HA	1:A:236:HIS:O	2.19	0.42
1:B:151:TRP:HA	1:B:247:VAL:HG13	2.03	0.40

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	103/107 (96%)	100 (97%)	3 (3%)	0	100	100
1	B	102/107 (95%)	97 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1/4 (25%)	1 (100%)	0	0	100	100
2	D	1/4 (25%)	1 (100%)	0	0	100	100
All	All	207/222 (93%)	199 (96%)	8 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	86/94 (92%)	85 (99%)	1 (1%)	74	85
1	B	85/94 (90%)	85 (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	173/190 (91%)	172 (99%)	1 (1%)	87	94

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

Mol	Chain	Res	Type
1	A	171	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	B	242	HIS

5.3.3 RNA [i](#)

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	FTY	C	101	2	14,18,19	1.57	3 (21%)	21,27,29	2.74	7 (33%)
2	FTY	D	101	2	14,18,19	1.41	1 (7%)	21,27,29	1.96	5 (23%)

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	FTY	C	101	2	-	0/10/21/23	0/1/1/1
2	FTY	D	101	2	-	0/10/21/23	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	101	FTY	P-O2P	-3.82	1.47	1.54
2	D	101	FTY	P-O2P	-3.50	1.48	1.54
2	C	101	FTY	P-O3P	-2.35	1.50	1.54
2	C	101	FTY	P-O1P	-2.31	1.46	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	101	FTY	F2-C1-F1	-7.33	97.47	106.73
2	D	101	FTY	F2-C1-F1	-4.79	100.68	106.73
2	C	101	FTY	F2-C1-CZ	-4.45	104.75	110.49
2	D	101	FTY	F1-C1-CZ	-3.28	106.27	110.49
2	C	101	FTY	CE2-CZ-C1	-3.27	116.89	119.84
2	C	101	FTY	CD1-CE1-CZ	-2.95	117.30	121.23
2	D	101	FTY	F2-C1-CZ	-2.87	106.80	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	101	FTY	P-C1-CZ	3.04	118.08	108.95
2	D	101	FTY	O3P-P-O2P	3.15	116.91	108.00
2	C	101	FTY	O3P-P-O2P	3.22	117.09	108.00
2	C	101	FTY	CE1-CZ-C1	3.99	123.45	119.84
2	C	101	FTY	P-C1-CZ	4.05	121.11	108.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	101	FTY	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	240:LEU	C	241:CYS	N	1.17

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, 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(Å ²)	Q<0.9
1	A	105/107 (98%)	-0.35	1 (0%) 82 81	7, 23, 46, 68	0
1	B	104/107 (97%)	-0.15	6 (5%) 23 22	9, 22, 57, 69	0
2	C	1/4 (25%)	-1.06	0 100 100	18, 18, 18, 18	0
2	D	1/4 (25%)	-0.82	0 100 100	24, 24, 24, 24	0
All	All	211/222 (95%)	-0.26	7 (3%) 46 44	7, 23, 56, 69	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	ALA	3.2
1	B	197	ALA	3.2
1	A	194	PHE	3.2
1	B	196	ASN	2.6
1	B	182	THR	2.2
1	B	194	PHE	2.1
1	B	195	ASP	2.0

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, 95th 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 ²)	Q<0.9
2	FTY	D	101	18/19	0.97	0.10	0,26,37,37	0
2	FTY	C	101	18/19	0.98	0.12	0,13,20,23	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.