

Full wwPDB X-ray Structure Validation Report (i)

Apr 19, 2021 – 04:02 pm BST

PDB ID : 2IUI

Title: Crystal structure of the PI3-kinase p85 N-terminal SH2 domain in complex

with PDGFR phosphotyrosyl peptide

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Deposited on : 2006-06-03

Resolution : 2.40 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 (i) symbol.

The following versions of software and data (see references (1)) 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)

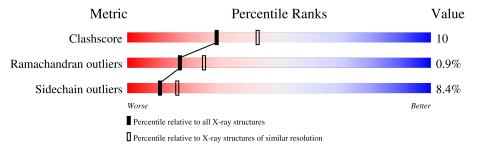
Validation Pipeline (wwPDB-VP) : 2.18

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 2.40 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	A	120	66%	20%	•• 11%
1	В	120	72%	16%	• • 8%
2	С	11	64%	36%	
2	D	11	73%	18%	9%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2087 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 Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	107	Total 879	C 550	N 152	O 166	S 2	0	0	0
	_			$\frac{333}{C}$		0	$\frac{2}{S}$			
1	В	110	903	571		172	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ASN	ASP	conflict	UNP P27986
В	1009	ASN	ASP	conflict	UNP P27986

• Molecule 2 is a protein called Platelet-derived growth factor receptor beta.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace			
9	С	11	Total	С	N	О	Р	S	0	0	0
		11	94	58	12	21	1	2	U	U	0
2	D	11	Total	С	N	О	Р	S	0	0	0
<u> </u>	D	11	94	58	12	21	1	2	U	U	U

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	202	ILE	VAL	$\operatorname{conflict}$	UNP P09619
D	1202	ILE	VAL	$\operatorname{conflict}$	UNP P09619

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	В	41	Total O 41 41	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	13	Total O 13 13	0	0
3	D	8	Total O 8 8	0	0

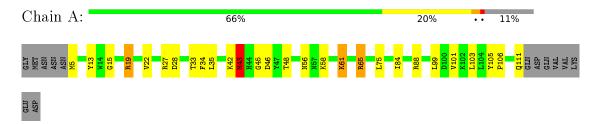


3 Residue-property plots (i)

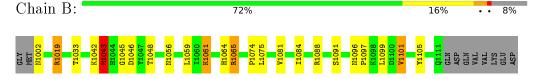
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Phosphatidylinositol 3-kinase regulatory subunit alpha



• Molecule 1: Phosphatidylinositol 3-kinase regulatory subunit alpha



• Molecule 2: Platelet-derived growth factor receptor beta

Chain C: 64% 36%



• Molecule 2: Platelet-derived growth factor receptor beta

Chain D: 73% 18% 9%





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	40.76Å 61.94Å 108.36Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	15.00 - 2.40	Depositor	
% Data completeness	(Not available) (15.00-2.40)	Depositor	
(in resolution range)	(1000 available) (10.00 2.40)	Depositor	
R_{merge}	0.06	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
R, R_{free}	0.178 , 0.248	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2087	wwPDB-VP	
Average B, all atoms (Å ²)	33.0	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: PTR

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).

Mal	Mol Chain		lengths	Bond angles		
MIOI	Chain	$\mid RMSZ \mid \# Z > 5$		RMSZ	# Z > 5	
1	A	0.48	0/899	0.60	0/1213	
1	В	0.45	0/923	0.58	0/1246	
2	С	0.49	0/77	0.54	0/99	
2	D	0.45	0/77	0.53	0/99	
All	All	0.47	0/1976	0.59	0/2657	

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	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	879	0	860	20	0
1	В	903	0	878	16	0
2	С	94	0	88	3	0
2	D	94	0	88	2	0
3	A	55	0	0	2	0
3	В	41	0	0	3	0
3	С	13	0	0	1	0
3	D	8	0	0	0	0
All	All	2087	0	1914	37	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 10.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:58:LYS:HB3	2:C:205:VAL:HG21	1.90	0.53
1:A:43:MET:SD	1:A:45:GLY:HA2	2.48	0.53
1:A:43:MET:SD	1:A:45:GLY:N	2.82	0.52
1:B:1033:THR:HA	1:B:1105:TYR:O	2.09	0.51
1:A:88:ARG:NH2	3:A:2041:HOH:O	2.44	0.50
1:B:1097:PRO:HA	3:B:2037:HOH:O	2.11	0.49
1:A:65:ARG:HB2	1:A:75:LEU:HD12	1.95	0.49
1:A:13:TYR:CZ	1:A:15:GLY:HA2	2.50	0.47
1:A:27:ARG:O	1:A:28:ASP:HB2	2.15	0.47
1:A:22:VAL:HG22	1:A:35:LEU:HD11	1.97	0.47
1:B:1045:GLY:HA3	1:B:1064:HIS:HD2	1.80	0.46
1:B:1019:ARG:HH21	1:B:1019:ARG:HG3	1.80	0.46
2:C:202:ILE:HB	3:C:2007:HOH:O	2.16	0.46
1:A:19:ARG:HH21	1:A:19:ARG:HG3	1.82	0.45
1:A:33:THR:HA	1:A:105:TYR:O	2.17	0.44
1:B:1043:MET:SD	1:B:1045:GLY:N	2.86	0.44
1:B:1084:ILE:O	1:B:1088:ARG:HG2	2.18	0.44
1:B:1042:LYS:HD2	1:B:1042:LYS:HA	1.84	0.44
1:B:1081:VAL:HG13	3:B:2028:HOH:O	2.16	0.44
1:A:65:ARG:HB2	1:A:75:LEU:CD1	2.48	0.43
1:A:99:LEU:HD11	2:C:205:VAL:HG11	2.00	0.43
1:A:34:PHE:CD2	1:A:103:LEU:HB3	2.53	0.43
1:A:106:PRO:HD2	3:A:2053:HOH:O	2.19	0.43
1:A:111:GLN:HG2	1:A:111:GLN:O	2.19	0.42
1:B:1091:SER:HA	1:B:1101:VAL:O	2.19	0.42
1:B:1048:THR:OG1	1:B:1061:LYS:NZ	2.52	0.42
1:B:1074:PRO:HD3	2:D:1211:LYS:HB3	2.02	0.42
1:A:34:PHE:CE2	1:A:103:LEU:HB3	2.55	0.42
1:A:42:LYS:HD2	1:A:42:LYS:HA	1.82	0.42
1:B:1059:LEU:HD11	3:B:2018:HOH:O	2.20	0.41
1:A:43:MET:SD	1:A:45:GLY:CA	3.08	0.41
1:B:1096:ASN:HA	1:B:1097:PRO:HD2	1.93	0.41
1:A:48:THR:OG1	1:A:61:LYS:NZ	2.53	0.41
1:A:84:ILE:O	1:A:88:ARG:HG2	2.20	0.41
1:B:1099:LEU:HD11	2:D:1205:VAL:HG11	2.02	0.41
1:B:1019:ARG:HG3	1:B:1019:ARG:NH2	2.35	0.41
1:B:1065:ARG:HB2	1:B:1075:LEU:HD12	2.03	0.41



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	Perce	\mathbf{ntiles}
1	A	105/120~(88%)	99 (94%)	5 (5%)	1 (1%)	15	23
1	В	$108/120 \; (90\%)$	102 (94%)	5 (5%)	1 (1%)	17	25
2	С	8/11 (73%)	7 (88%)	1 (12%)	0	100	100
2	D	8/11~(73%)	7 (88%)	1 (12%)	0	100	100
All	All	$229/262 \; (87\%)$	215 (94%)	12 (5%)	2 (1%)	17	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	${f Res}$	Type
1	A	43	MET
1	В	1043	MET

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	96/108 (89%)	88 (92%)	8 (8%)	11 17
1	В	99/108 (92%)	91 (92%)	8 (8%)	11 18
2	С	10/10 (100%)	9 (90%)	1 (10%)	7 11
2	D	10/10 (100%)	9 (90%)	1 (10%)	7 11
All	All	215/236 (91%)	197 (92%)	18 (8%)	11 16



All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	19	ARG
1	A	43	MET
1	A	46	ASP
1	A	56	ASN
1	A	61	LYS
1	A	65	ARG
1	A	101	VAL
1	В	1002	ASN
1	В	1019	ARG
1	В	1043	MET
1	В	1046	ASP
1	В	1056	ASN
1	В	1061	LYS
1	В	1065	ARG
1	В	1101	VAL
2	С	211	LYS
2	D	1211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	89	ASN
1	В	1002	ASN
1	В	1064	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	Tuno	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	$\mid \# Z > 2 \mid$
2	PTR	D	1204	2	15,16,17	1.69	3 (20%)	19,22,24	1.24	2 (10%)
2	PTR	С	204	2	15,16,17	0.90	0	19,22,24	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
2	PTR	D	1204	2	-	2/10/11/13	0/1/1/1
2	PTR	С	204	2	-	1/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed(\AA)}$	$\operatorname{Ideal}(ext{\AA})$
2	D	1204	PTR	P-O3P	-3.68	1.40	1.54
2	D	1204	PTR	P-OH	-3.49	1.53	1.59
2	D	1204	PTR	P-O2P	-3.44	1.41	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
2	D	1204	PTR	O2P-P-O1P	3.68	125.07	110.68
2	С	204	PTR	O3P-P-O2P	2.33	116.53	107.64
2	D	1204	PTR	O3P-P-O1P	-2.19	102.11	110.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1204	PTR	N-CA-CB-CG
2	С	204	PTR	C-CA-CB-CG
2	D	1204	PTR	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.



5.5 Carbohydrates (i)

There are no monosaccharides 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

