Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 06:48 AM EDT

PDB ID	:	2REA
Title	:	Crystal structures of C2ALPHA-PI3 kinase PX-domain domain indicate conformational change associated with ligand binding.
Authors	:	Parkinson, G.N.; Vines, D.; Driscoll, P.C.; Djordjevic, S.
Deposited on	:	2007-09-26
Resolution	:	2.50 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

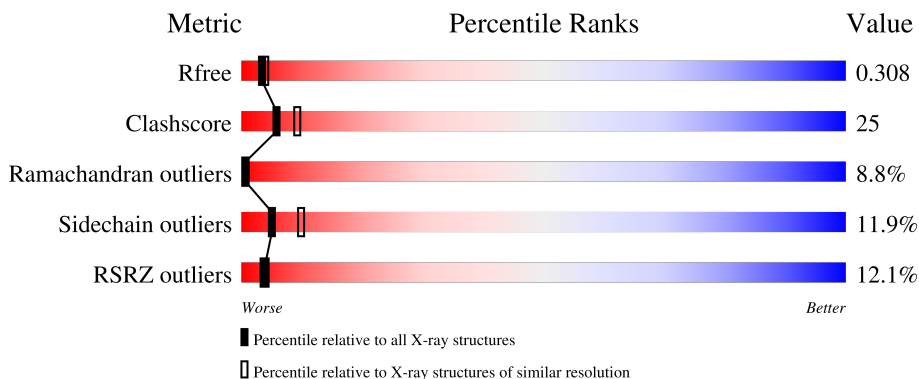|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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	Percentile Ranks	Value
Rfree		0.308
Clashscore		25
Ramachandran outliers		8.8%
Sidechain outliers		11.9%
RSRZ outliers		12.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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% 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	121	12% 47% 33% 12% • •

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 964 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-4-phosphate 3-kinase C2 domain-containing alpha polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total 945	C 611	N 164	O 166	S 4	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1420	MET	-	expression tag	UNP O00443
A	1533	GLY	-	expression tag	UNP O00443
A	1534	SER	-	expression tag	UNP O00443
A	1535	HIS	-	expression tag	UNP O00443
A	1536	HIS	-	expression tag	UNP O00443
A	1537	HIS	-	expression tag	UNP O00443
A	1538	HIS	-	expression tag	UNP O00443
A	1539	HIS	-	expression tag	UNP O00443
A	1540	HIS	-	expression tag	UNP O00443

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total 19	O 19	0	0

3 Residue-property plots ⓘ

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 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: Phosphatidylinositol-4-phosphate 3-kinase C2 domain-containing alpha polypeptide
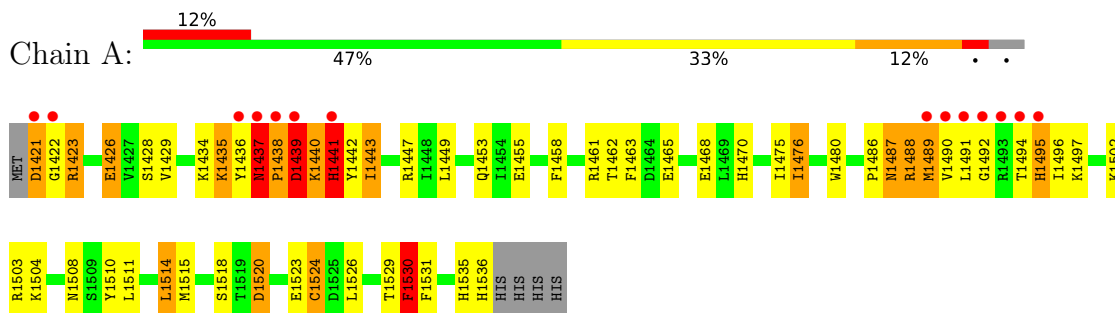
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	56.87Å 56.87Å 93.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.19 – 2.50 27.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.3 (27.19-2.50) 89.3 (27.19-2.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.00 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.231 , 0.318 0.225 , 0.308	Depositor DCC
R_{free} test set	250 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	964	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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	1.54	7/971 (0.7%)	1.40	7/1311 (0.5%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1468	GLU	CB-CG	7.24	1.66	1.52
1	A	1504	LYS	CE-NZ	6.63	1.65	1.49
1	A	1524	CYS	CB-SG	-5.95	1.72	1.81
1	A	1468	GLU	CG-CD	5.40	1.60	1.51
1	A	1458	PHE	CE2-CZ	5.39	1.47	1.37
1	A	1421	ASP	CB-CG	5.28	1.62	1.51
1	A	1530	PHE	CD2-CE2	-5.00	1.29	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1441	HIS	C-N-CA	-7.80	102.20	121.70
1	A	1443	ILE	CG1-CB-CG2	-7.24	95.47	111.40
1	A	1503	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	A	1421	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	1447	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	1514	LEU	CA-CB-CG	5.40	127.73	115.30
1	A	1442	TYR	N-CA-C	5.08	124.71	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1437	ASN	Peptide

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	945	0	913	47	0
2	A	19	0	0	2	0
All	All	964	0	913	47	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 25.

All (47) 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:1487:ASN:HD22	1:A:1487:ASN:N	1.34	1.17
1:A:1487:ASN:N	1:A:1487:ASN:ND2	2.10	0.96
1:A:1488:ARG:HD3	1:A:1502:LYS:HZ3	1.35	0.90
1:A:1421:ASP:HB2	1:A:1523:GLU:OE2	1.74	0.87
1:A:1423:ARG:HG3	2:A:1552:HOH:O	1.80	0.80
1:A:1435:LYS:HD2	1:A:1437:ASN:OD1	1.82	0.80
1:A:1488:ARG:HD3	1:A:1502:LYS:NZ	1.99	0.78
1:A:1487:ASN:HD22	1:A:1487:ASN:H	1.26	0.76
1:A:1470:HIS:HD2	1:A:1510:TYR:OH	1.72	0.73
1:A:1440:LYS:HB3	1:A:1441:HIS:HA	1.73	0.71
1:A:1426:GLU:HG3	1:A:1449:LEU:HD23	1.71	0.71
1:A:1486:PRO:C	1:A:1487:ASN:HD22	1.96	0.68
1:A:1453:GLN:OE1	1:A:1455:GLU:O	2.13	0.67
1:A:1488:ARG:HH11	1:A:1502:LYS:HZ3	1.44	0.65
1:A:1422:GLY:O	1:A:1423:ARG:C	2.36	0.64
1:A:1461:ARG:HA	1:A:1465:GLU:OE2	2.01	0.60
1:A:1435:LYS:CD	1:A:1437:ASN:OD1	2.48	0.59
1:A:1497:LYS:NZ	1:A:1497:LYS:HB3	2.17	0.58
1:A:1434:LYS:HG2	1:A:1434:LYS:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1529:THR:O	1:A:1530:PHE:C	2.42	0.57
1:A:1426:GLU:CG	1:A:1449:LEU:HD23	2.35	0.56
1:A:1440:LYS:CB	1:A:1441:HIS:HA	2.35	0.56
1:A:1426:GLU:OE2	1:A:1449:LEU:HD23	2.06	0.55
1:A:1487:ASN:ND2	1:A:1487:ASN:H	1.93	0.55
1:A:1476:ILE:HD11	1:A:1526:LEU:HD12	1.91	0.53
1:A:1470:HIS:CD2	1:A:1510:TYR:OH	2.58	0.51
1:A:1426:GLU:OE2	1:A:1449:LEU:CD2	2.59	0.50
1:A:1428:SER:HA	1:A:1508:ASN:ND2	2.26	0.50
1:A:1529:THR:O	1:A:1531:PHE:N	2.44	0.50
1:A:1488:ARG:HH11	1:A:1502:LYS:NZ	2.12	0.47
1:A:1462:THR:O	1:A:1463:PHE:C	2.53	0.46
1:A:1480:TRP:O	1:A:1480:TRP:CE3	2.69	0.46
1:A:1535:HIS:HE1	2:A:1545:HOH:O	1.99	0.46
1:A:1520:ASP:O	1:A:1524:CYS:HB3	2.17	0.45
1:A:1497:LYS:HB3	1:A:1497:LYS:HZ2	1.81	0.44
1:A:1438:PRO:HB2	1:A:1439:ASP:OD1	2.19	0.43
1:A:1434:LYS:O	1:A:1434:LYS:CG	2.66	0.43
1:A:1494:THR:HA	1:A:1495:HIS:CB	2.48	0.42
1:A:1535:HIS:O	1:A:1536:HIS:HB2	2.19	0.42
1:A:1510:TYR:CE2	1:A:1514:LEU:HD22	2.55	0.42
1:A:1429:VAL:H	1:A:1508:ASN:HD22	1.68	0.41
1:A:1475:ILE:HG23	1:A:1475:ILE:HD12	1.79	0.41
1:A:1443:ILE:HD13	1:A:1443:ILE:HG23	1.45	0.41
1:A:1443:ILE:HG21	1:A:1443:ILE:HD12	1.67	0.41
1:A:1490:VAL:O	1:A:1491:LEU:C	2.59	0.41
1:A:1511:LEU:O	1:A:1515:MET:HG2	2.21	0.41
1:A:1488:ARG:CD	1:A:1502:LYS:HZ3	2.18	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	114/121 (94%)	88 (77%)	16 (14%)	10 (9%)	1 0

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1423	ARG
1	A	1435	LYS
1	A	1495	HIS
1	A	1496	ILE
1	A	1489	MET
1	A	1530	PHE
1	A	1438	PRO
1	A	1437	ASN
1	A	1492	GLY
1	A	1439	ASP

5.3.2 Protein sidechains ⓘ

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	101/112 (90%)	89 (88%)	12 (12%)	5 10

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1426	GLU
1	A	1436	TYR
1	A	1437	ASN
1	A	1439	ASP
1	A	1440	LYS
1	A	1441	HIS
1	A	1476	ILE
1	A	1487	ASN
1	A	1488	ARG
1	A	1489	MET
1	A	1518	SER

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Mol	Chain	Res	Type
1	A	1520	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1453	GLN
1	A	1470	HIS
1	A	1487	ASN
1	A	1508	ASN
1	A	1512	GLN
1	A	1535	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	116/121 (95%)	0.15	14 (12%)	4	4	16, 35, 80, 80	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1493	ARG	6.3
1	A	1492	GLY	5.8
1	A	1491	LEU	4.8
1	A	1494	THR	4.8
1	A	1421	ASP	4.2
1	A	1495	HIS	4.1
1	A	1438	PRO	3.9
1	A	1490	VAL	3.7
1	A	1489	MET	3.6
1	A	1437	ASN	3.5
1	A	1436	TYR	3.4
1	A	1441	HIS	2.5
1	A	1439	ASP	2.4
1	A	1422	GLY	2.4

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.