



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 04:45 pm BST

PDB ID : 2RED
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 : 2.10 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

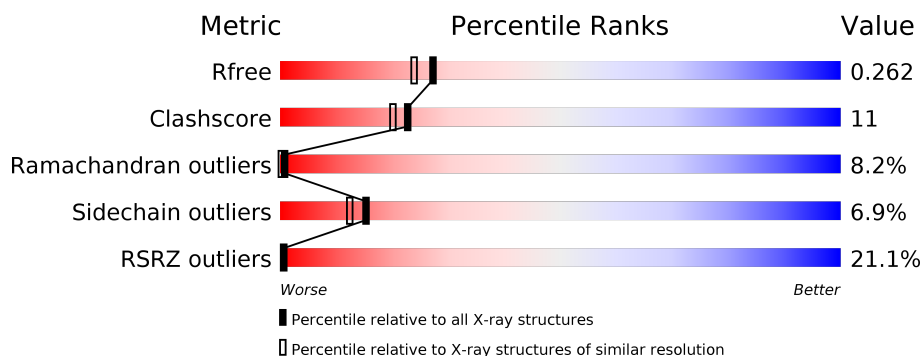
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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 $\leq 5\%$. 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	303	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1063 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	114	Total	C	N	O	S	0	0	0
			935	605	161	164	5			

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 GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

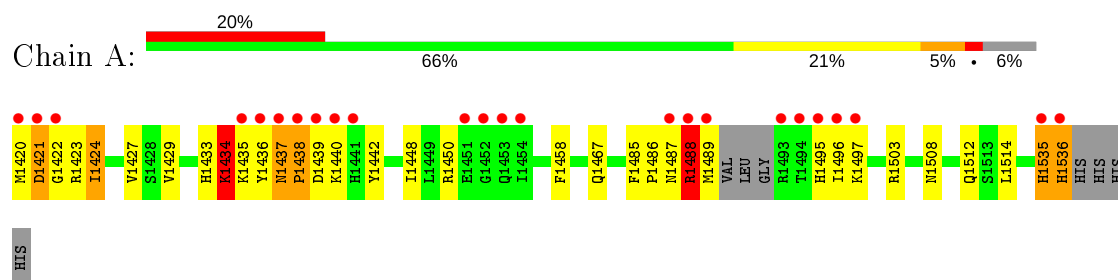
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		

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: 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	56.55Å 56.55Å 92.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.27 – 2.10 28.28 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (28.27-2.10) 98.9 (28.28-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.16 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.235 , 0.274 0.224 , 0.262	Depositor DCC
R_{free} test set	539 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1063	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0/960	0.87	0/1295

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1535	HIS	Peptide

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	935	0	903	22	0
2	A	36	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	92	0	0	2	0
All	All	1063	0	951	22	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 11.

All (22) 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:1429:VAL:H	1:A:1508:ASN:HD22	1.36	0.72
1:A:1442:TYR:HE1	1:A:1497:LYS:HE3	1.61	0.65
1:A:1535:HIS:O	1:A:1536:HIS:HB2	1.98	0.64
1:A:1433:HIS:O	1:A:1434:LYS:HB2	1.98	0.63
1:A:1424:ILE:HD12	1:A:1450:ARG:HG2	1.82	0.61
1:A:1489:MET:HA	1:A:1503:ARG:HH22	1.67	0.59
1:A:1436:TYR:O	1:A:1437:ASN:HB2	2.06	0.56
1:A:1467:GLN:HE22	1:A:1487:ASN:ND2	2.03	0.56
1:A:1442:TYR:CE1	1:A:1497:LYS:HE3	2.44	0.51
1:A:1421:ASP:HB2	3:A:39:HOH:O	2.10	0.51
1:A:1427:VAL:HG23	1:A:1448:ILE:HD13	1.94	0.50
1:A:1488:ARG:HB3	1:A:1503:ARG:HH21	1.75	0.49
1:A:1423:ARG:NH1	3:A:52:HOH:O	2.18	0.49
1:A:1436:TYR:O	1:A:1437:ASN:CB	2.60	0.48
1:A:1440:LYS:HA	1:A:1440:LYS:HE2	1.95	0.48
1:A:1429:VAL:H	1:A:1508:ASN:ND2	2.08	0.48
1:A:1535:HIS:O	1:A:1536:HIS:CB	2.63	0.46
1:A:1438:PRO:O	1:A:1440:LYS:N	2.51	0.43
1:A:1434:LYS:NZ	1:A:1440:LYS:HB3	2.34	0.43
1:A:1485:PHE:CD1	1:A:1486:PRO:HD2	2.54	0.42
1:A:1508:ASN:O	1:A:1512:GLN:HG2	2.21	0.41
1:A:1458:PHE:HE1	2:A:305:GOL:H31	1.86	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	110/121 (91%)	97 (88%)	4 (4%)	9 (8%)	1	0

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1422	GLY
1	A	1434	LYS
1	A	1435	LYS
1	A	1438	PRO
1	A	1439	ASP
1	A	1488	ARG
1	A	1496	ILE
1	A	1437	ASN
1	A	1495	HIS

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%)	94 (93%)	7 (7%)	15	12

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1420	MET
1	A	1421	ASP
1	A	1424	ILE
1	A	1434	LYS
1	A	1488	ARG
1	A	1514	LEU
1	A	1536	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1433	HIS
1	A	1467	GLN
1	A	1470	HIS
1	A	1487	ASN
1	A	1508	ASN
1	A	1512	GLN
1	A	1516	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands 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	GOL	A	303	-	5,5,5	0.50	0	5,5,5	0.26	0
2	GOL	A	304	-	5,5,5	0.33	0	5,5,5	0.39	0
2	GOL	A	305	-	5,5,5	0.57	0	5,5,5	0.37	0
2	GOL	A	306	-	5,5,5	0.36	0	5,5,5	0.14	0
2	GOL	A	301	-	5,5,5	0.36	0	5,5,5	0.13	0
2	GOL	A	302	-	5,5,5	0.37	0	5,5,5	0.24	0

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	GOL	A	303	-	-	2/4/4/4	-
2	GOL	A	304	-	-	4/4/4/4	-
2	GOL	A	305	-	-	2/4/4/4	-
2	GOL	A	306	-	-	4/4/4/4	-
2	GOL	A	301	-	-	4/4/4/4	-
2	GOL	A	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	303	GOL	O1-C1-C2-C3
2	A	304	GOL	C1-C2-C3-O3
2	A	304	GOL	O2-C2-C3-O3
2	A	306	GOL	O1-C1-C2-C3
2	A	301	GOL	C1-C2-C3-O3
2	A	301	GOL	O2-C2-C3-O3
2	A	304	GOL	O1-C1-C2-C3
2	A	305	GOL	C1-C2-C3-O3
2	A	306	GOL	C1-C2-C3-O3
2	A	301	GOL	O1-C1-C2-C3
2	A	302	GOL	C1-C2-C3-O3
2	A	303	GOL	O1-C1-C2-O2
2	A	305	GOL	O2-C2-C3-O3
2	A	306	GOL	O2-C2-C3-O3
2	A	304	GOL	O1-C1-C2-O2
2	A	306	GOL	O1-C1-C2-O2
2	A	301	GOL	O1-C1-C2-O2
2	A	302	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	305	GOL	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

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	114/121 (94%)	1.69	24 (21%) 1 0	15, 28, 76, 80	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1436	TYR	13.2
1	A	1435	LYS	9.3
1	A	1420	MET	9.2
1	A	1494	THR	9.1
1	A	1493	ARG	9.0
1	A	1438	PRO	8.0
1	A	1489	MET	7.6
1	A	1496	ILE	7.2
1	A	1437	ASN	7.1
1	A	1495	HIS	7.1
1	A	1439	ASP	6.9
1	A	1536	HIS	6.1
1	A	1421	ASP	5.3
1	A	1488	ARG	5.1
1	A	1422	GLY	4.4
1	A	1497	LYS	3.7
1	A	1454	ILE	3.7
1	A	1453	GLN	3.6
1	A	1441	HIS	3.6
1	A	1535	HIS	3.4
1	A	1451	GLU	3.0
1	A	1440	LYS	2.9
1	A	1487	ASN	2.2
1	A	1452	GLY	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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(\AA^2)	Q<0.9
2	GOL	A	306	6/6	0.66	0.39	74,76,76,78	0
2	GOL	A	301	6/6	0.72	0.38	80,80,80,80	0
2	GOL	A	302	6/6	0.74	0.24	67,68,68,69	0
2	GOL	A	303	6/6	0.80	0.47	80,80,80,80	0
2	GOL	A	304	6/6	0.82	0.23	62,64,66,69	0
2	GOL	A	305	6/6	0.95	0.13	36,38,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.