



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2017 – 03:53 PM EDT

PDB ID : 2A98
Title : Crystal structure of the catalytic domain of human inositol 1,4,5-trisphosphate 3-kinase C
Authors : Hallberg, B.M.; Ogg, D.; Ehn, M.; Graslund, S.; Hammarstrom, M.; Kotenyova, T.; Nilsson-Ehle, P.; Nordlund, P.; Persson, C.; Sagemark, J.; Schuler, H.; Stenmark, P.; Thorsell, A.-G.; Arrowsmith, C.; Edwards, A.; Sundstrom, M.; Weigelt, J.; Structural Genomics Consortium (SGC)
Deposited on : unknown
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
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-20030345

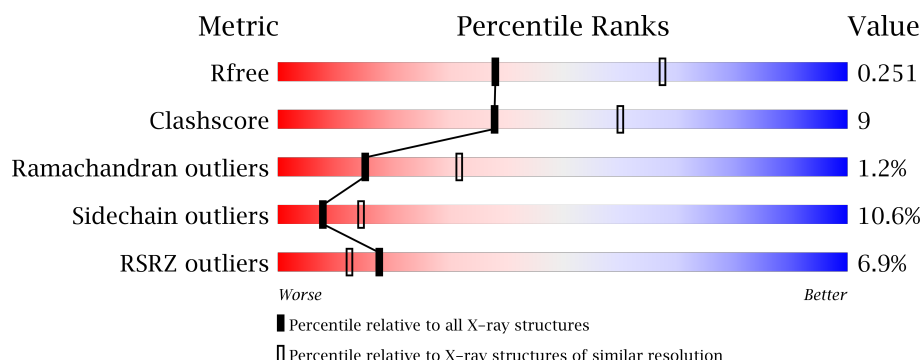
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	259	

2 Entry composition [i](#)

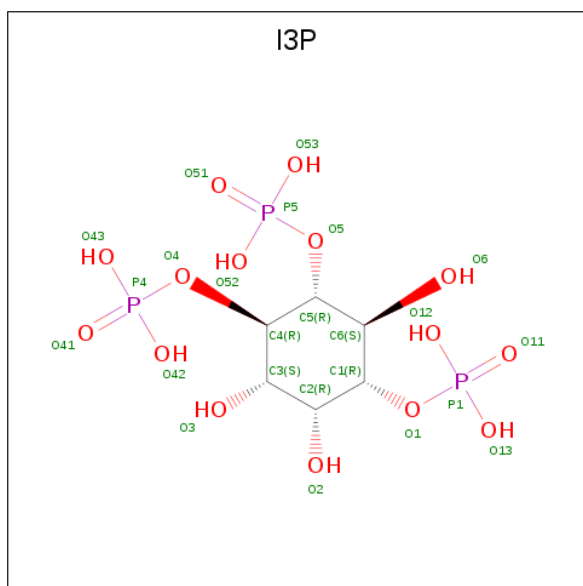
There are 2 unique types of molecules in this entry. The entry contains 2099 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Inositol 1,4,5-trisphosphate 3-kinase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	259	2075	1309	357	392	17	0	0	0

- Molecule 2 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).

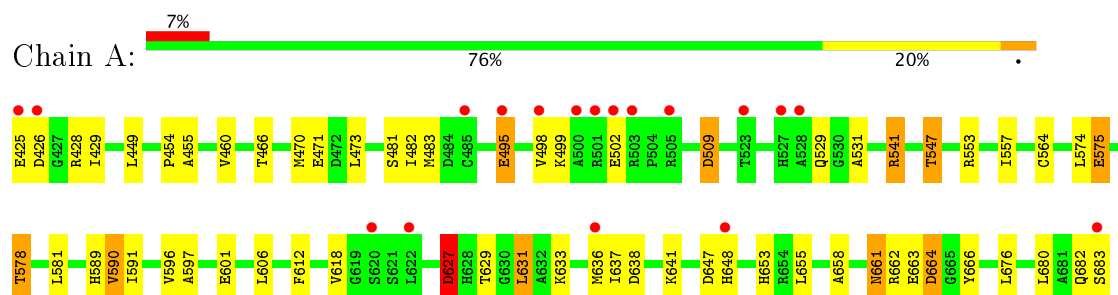


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	24	6	15	3	0	0

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: Inositol 1,4,5-trisphosphate 3-kinase C



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.72Å 87.72Å 174.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.68 – 2.60 28.33 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.68-2.60) 99.9 (28.33-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.262 0.208 , 0.251	Depositor DCC
R_{free} test set	629 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 11.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2099	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: I3P

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	1.19	2/2120 (0.1%)	0.88	7/2860 (0.2%)

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	1	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	502	GLU	CD-OE1	33.43	1.62	1.25
1	A	502	GLU	CD-OE2	23.71	1.51	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	GLU	OE1-CD-OE2	8.40	133.39	123.30
1	A	627	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	A	627	ASP	CB-CA-C	-5.89	98.62	110.40
1	A	631	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	502	GLU	CG-CD-OE2	-5.83	106.64	118.30
1	A	590	VAL	CB-CA-C	5.64	122.12	111.40
1	A	683	SER	N-CA-C	5.48	125.79	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	590	VAL	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	589	HIS	Peptide
1	A	682	GLN	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	2075	0	2039	36	0
2	A	24	0	9	0	0
All	All	2099	0	2048	36	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 9.

All (36) 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:541:ARG:HG2	1:A:541:ARG:HH11	1.18	1.05
1:A:547:THR:HG21	1:A:553:ARG:HH11	1.39	0.87
1:A:547:THR:HG22	1:A:553:ARG:HD3	1.55	0.87
1:A:547:THR:CG2	1:A:553:ARG:HD3	2.12	0.80
1:A:541:ARG:HG2	1:A:541:ARG:NH1	1.92	0.74
1:A:495:GLU:HA	1:A:498:VAL:HG12	1.69	0.74
1:A:495:GLU:O	1:A:499:LYS:HB2	1.92	0.69
1:A:449:LEU:HD22	1:A:636:MET:HE2	1.74	0.69
1:A:483:MET:HE2	1:A:557:ILE:HD11	1.74	0.68
1:A:454:PRO:HB3	1:A:473:LEU:HD21	1.80	0.63
1:A:574:LEU:O	1:A:578:THR:HG23	1.99	0.62
1:A:597:ALA:O	1:A:601:GLU:HG2	2.02	0.59
1:A:664:ASP:HB3	1:A:666:TYR:H	1.66	0.59
1:A:547:THR:CG2	1:A:553:ARG:HH11	2.14	0.57
1:A:547:THR:HG21	1:A:553:ARG:NH1	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ASN:HD22	1:A:662:ARG:N	2.08	0.52
1:A:658:ALA:H	1:A:661:ASN:ND2	2.08	0.52
1:A:557:ILE:O	1:A:564:CYS:HB2	2.10	0.52
1:A:653:HIS:CE1	1:A:664:ASP:OD2	2.64	0.51
1:A:483:MET:HE1	1:A:581:LEU:HD23	1.92	0.50
1:A:653:HIS:ND1	1:A:664:ASP:OD2	2.45	0.49
1:A:483:MET:CE	1:A:557:ILE:HD11	2.40	0.49
1:A:449:LEU:HD22	1:A:636:MET:CE	2.43	0.48
1:A:612:PHE:CE2	1:A:653:HIS:CD2	3.02	0.47
1:A:637:ILE:O	1:A:638:ASP:HB2	2.14	0.47
1:A:574:LEU:O	1:A:578:THR:CG2	2.64	0.45
1:A:481:SER:C	1:A:482:ILE:HG13	2.38	0.44
1:A:661:ASN:ND2	1:A:663:GLU:H	2.15	0.44
1:A:575:GLU:OE2	1:A:575:GLU:N	2.34	0.44
1:A:627:ASP:HB3	1:A:629:THR:H	1.83	0.44
1:A:529:GLN:HE21	1:A:531:ALA:HB3	1.82	0.43
1:A:429:ILE:HG22	1:A:470:MET:HB2	2.00	0.42
1:A:449:LEU:HD21	1:A:606:LEU:HD23	2.01	0.41
1:A:575:GLU:H	1:A:575:GLU:CD	2.22	0.41
1:A:455:ALA:HB3	1:A:471:GLU:HB2	2.03	0.41
1:A:541:ARG:CG	1:A:541:ARG:NH1	2.74	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	257/259 (99%)	247 (96%)	7 (3%)	3 (1%)	15	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	ASP
1	A	590	VAL
1	A	647	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	226/226 (100%)	202 (89%)	24 (11%)	8 14

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	425	GLU
1	A	426	ASP
1	A	428	ARG
1	A	460	VAL
1	A	466	THR
1	A	495	GLU
1	A	509	ASP
1	A	541	ARG
1	A	547	THR
1	A	575	GLU
1	A	578	THR
1	A	591	ILE
1	A	596	VAL
1	A	618	VAL
1	A	627	ASP
1	A	631	LEU
1	A	633	LYS
1	A	641	LYS
1	A	648	HIS
1	A	655	LEU
1	A	661	ASN
1	A	664	ASP
1	A	676	LEU
1	A	680	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	A	529	GLN
1	A	572	GLN
1	A	661	ASN
1	A	678	GLN

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](#)

1 ligand is 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	I3P	A	1	-	24,24,24	1.06	3 (12%)	36,39,39	1.20	4 (11%)

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	I3P	A	1	-	-	0/15/39/39	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	I3P	P4-O4	2.32	1.63	1.59
2	A	1	I3P	P5-O5	2.57	1.64	1.59
2	A	1	I3P	P1-O1	2.60	1.64	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	I3P	O1-P1-O11	-2.30	100.24	109.26
2	A	1	I3P	O5-P5-O51	-2.19	100.69	109.26
2	A	1	I3P	O1-C1-C6	-2.03	103.91	108.66
2	A	1	I3P	C3-C2-C1	2.10	113.96	109.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	259/259 (100%)	0.17	18 (6%)	18 12	26, 32, 37, 40	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	VAL	4.7
1	A	503	ARG	4.5
1	A	683	SER	3.9
1	A	426	ASP	3.8
1	A	505	ARG	3.2
1	A	495	GLU	2.9
1	A	502	GLU	2.7
1	A	500	ALA	2.7
1	A	648	HIS	2.7
1	A	528	ALA	2.7
1	A	622	LEU	2.4
1	A	501	ARG	2.4
1	A	485	CYS	2.4
1	A	620	SER	2.4
1	A	636	MET	2.3
1	A	527	HIS	2.2
1	A	523	THR	2.2
1	A	425	GLU	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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	I3P	A	1	24/24	0.94	0.14	-1.03	48,54,57,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.