

wwPDB X-ray Structure Validation Summary Report (i)

Dec 18, 2023 – 02:44 am GMT

PDB ID : 4D28

Title: Crystal structure of the kinase domain of CIPK24/SOS2

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Deposited on : 2014-05-08

Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$

EDS: 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

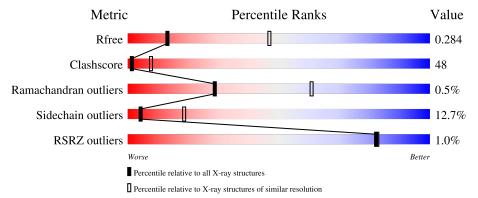
 $\begin{tabular}{lll} Validation Pipeline (wwPDB-VP) & : & 2.36 \end{tabular}$

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 3.30 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	446	27%	31%	·	39%			
1	В	446	25%	31%	7%	38%			
1	С	446	24%	33%	5%	37%			
1	D	446	21%	35%	5%	39%			



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8821 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 CBL-INTERACTING SERINE/THREONINE-PROTEIN KINASE 24.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	274	Total	С	N	О	S	0	0	0
1	A	214	2192	1404	382	399	7	0	U	
1	В	277	Total	С	N	О	S	0	0	0
1	Б	211	2217	1419	388	403	7	0	U	U
1	C	279	Total	С	N	О	S	0	0	0
1		219	2234	1430	390	407	7	0	U	
1	D	971	Total	С	N	О	S	0	0	0
1	ש	D 271		1397	379	395	7		U	U

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	LYS	PRO	engineered mutation	UNP Q9LDI3
A	107	LYS	GLU	engineered mutation	UNP Q9LDI3
A	109	ASP	SER	engineered mutation	UNP Q9LDI3
A	127	SER	CYS	engineered mutation	UNP Q9LDI3
A	167	ASN	ARG	conflict	UNP Q9LDI3
A	168	ASP	THR	engineered mutation	UNP Q9LDI3
A	228	ASP	SER	engineered mutation	UNP Q9LDI3
A	266	LYS	LEU	engineered mutation	UNP Q9LDI3
В	81	LYS	PRO	engineered mutation	UNP Q9LDI3
В	107	LYS	GLU	engineered mutation	UNP Q9LDI3
В	109	ASP	SER	engineered mutation	UNP Q9LDI3
В	127	SER	CYS	engineered mutation	UNP Q9LDI3
В	167	ASN	ARG	conflict	UNP Q9LDI3
В	168	ASP	THR	engineered mutation	UNP Q9LDI3
В	228	ASP	SER	engineered mutation	UNP Q9LDI3
В	266	LYS	LEU	engineered mutation	UNP Q9LDI3
С	81	LYS	PRO	engineered mutation	UNP Q9LDI3
С	107	LYS	GLU	engineered mutation	UNP Q9LDI3
С	109	ASP	SER	engineered mutation	UNP Q9LDI3
С	127	SER	CYS	engineered mutation	UNP Q9LDI3

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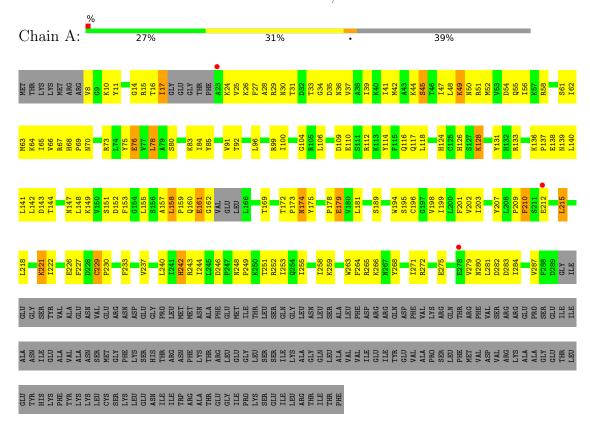
Chain	Residue	Modelled	Actual	Comment	Reference
С	167	ASN	ARG	conflict	UNP Q9LDI3
С	168	ASP	THR	engineered mutation	UNP Q9LDI3
С	228	ASP	SER	engineered mutation	UNP Q9LDI3
С	266	LYS	LEU	engineered mutation	UNP Q9LDI3
D	81	LYS	PRO	engineered mutation	UNP Q9LDI3
D	107	LYS	GLU	engineered mutation	UNP Q9LDI3
D	109	ASP	SER	engineered mutation	UNP Q9LDI3
D	127	SER	CYS	engineered mutation	UNP Q9LDI3
D	167	ASN	ARG	conflict	UNP Q9LDI3
D	168	ASP	THR	engineered mutation	UNP Q9LDI3
D	228	ASP	SER	engineered mutation	UNP Q9LDI3
D	266	LYS	LEU	engineered mutation	UNP Q9LDI3



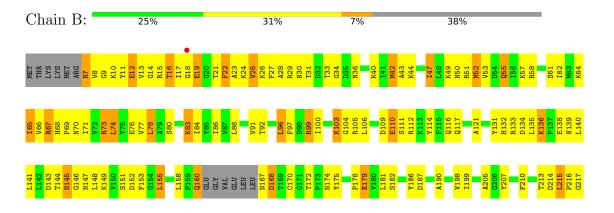
3 Residue-property plots (i)

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 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.

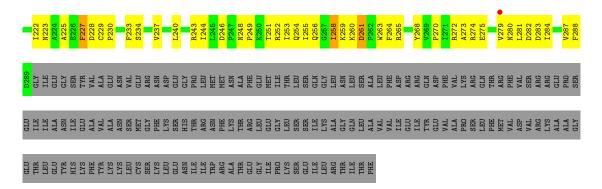
• Molecule 1: CBL-INTERACTING SERINE/THREONINE-PROTEIN KINASE 24



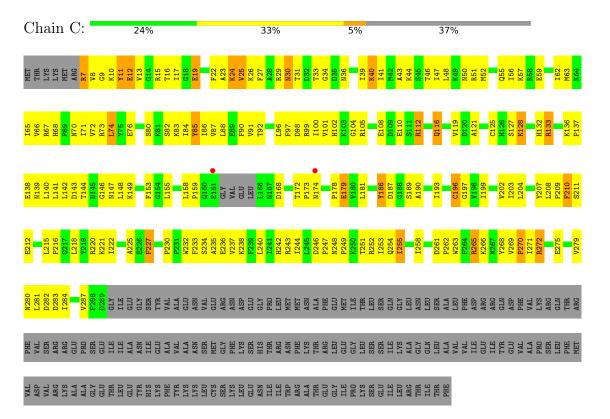
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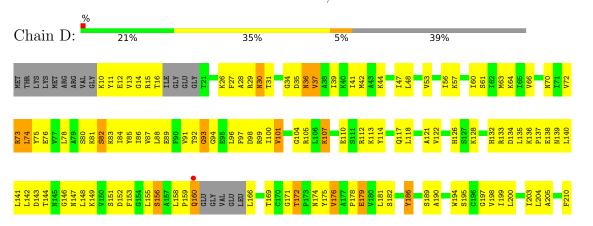




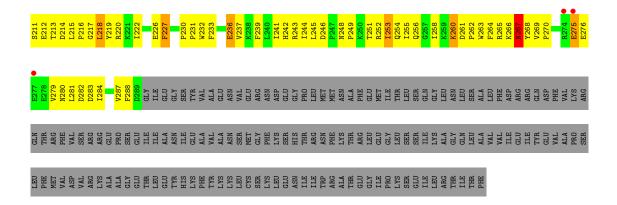
• Molecule 1: CBL-INTERACTING SERINE/THREONINE-PROTEIN KINASE 24



• Molecule 1: CBL-INTERACTING SERINE/THREONINE-PROTEIN KINASE 24









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	69.11Å 71.35Å 77.83Å	D
a, b, c, α , β , γ	104.85° 100.32° 118.96°	Depositor
Resolution (Å)	70.23 - 3.30	Depositor
Resolution (A)	70.23 - 3.30	EDS
% Data completeness	90.8 (70.23-3.30)	Depositor
(in resolution range)	90.8 (70.23-3.30)	EDS
R_{merge}	0.27	Depositor
R_{sum}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.73 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
P. P.	0.271 , 0.283	Depositor
R, R_{free}	0.275 , 0.284	DCC
R_{free} test set	810 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	72.5	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 20.6	EDS
L-test for twinning ²	$< L >=0.44, < L^2>=0.26$	Xtriage
	0.045 for k,h,-h-k-l	
Estimated twinning fraction	0.043 for -k,-h,-l	Xtriage
	0.069 for -h,-k,h+k+l	
F_o, F_c correlation	0.87	EDS
Total number of atoms	8821	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.13% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.30	0/2236	0.56	0/3020	
1	В	0.31	0/2263	0.56	0/3057	
1	С	0.29	0/2280	0.54	0/3080	
1	D	0.30	0/2223	0.54	0/3003	
All	All	0.30	0/9002	0.55	0/12160	

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	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2192	0	2222	171	0
1	В	2217	0	2244	202	0
1	С	2234	0	2261	241	0
1	D	2178	0	2206	254	0
All	All	8821	0	8933	860	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 48.

The worst 5 of 860 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:C:174:ASN:OD1	1:C:212:GLU:OE2	1.60	1.15
1:D:86:ILE:HG22	1:D:88:LEU:HD11	1.17	1.14
1:B:92:THR:OG1	1:B:144:THR:HG23	1.49	1.12
1:B:7:ARG:HD2	1:B:12:GLU:OE2	1.48	1.11
1:D:175:TYR:O	1:D:194:TRP:NE1	1.83	1.10

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	entiles
1	A	268/446~(60%)	254 (95%)	14 (5%)	0	100	100
1	В	273/446 (61%)	249 (91%)	23 (8%)	1 (0%)	34	66
1	C	275/446~(62%)	263 (96%)	11 (4%)	1 (0%)	34	66
1	D	265/446~(59%)	247 (93%)	15 (6%)	3 (1%)	14	45
All	All	1081/1784 (61%)	1013 (94%)	63 (6%)	5 (0%)	29	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	93	GLY
1	В	23	ALA
1	D	176	VAL
1	D	267	ASN
1	С	270	PRO

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	${\rm sidechain}$	conformation	was
analysed, and the total	number of	residues	S.						

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	A	239/388 (62%)	217 (91%)	22 (9%)	9	31
1	В	$241/388 \ (62\%)$	198 (82%)	43 (18%)	2	8
1	С	243/388 (63%)	214 (88%)	29 (12%)	5	21
1	D	238/388 (61%)	210 (88%)	28 (12%)	5	21
All	All	961/1552~(62%)	839 (87%)	122 (13%)	4	19

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	213	THR
1	D	179	GLU
1	С	25	VAL
1	D	174	ASN
1	D	253	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	256	GLN
1	D	102	HIS
1	С	139	ASN
1	D	126	HIS
1	A	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 (i)

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

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)

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, 95^{th} 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>	#RSF	RZ>	-2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	274/446 (61%)	-0.25	3 (1%) 8	80	81	40, 61, 100, 124	0
1	В	277/446 (62%)	-0.20	2 (0%) 8	87	88	39, 64, 125, 146	0
1	С	279/446 (62%)	-0.17	2 (0%) 8	87	88	44, 65, 121, 136	0
1	D	271/446 (60%)	-0.23	4 (1%)	73	72	47, 67, 109, 132	0
All	All	1101/1784 (61%)	-0.21	11 (0%)	82	82	39, 64, 116, 146	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	18	GLY	3.7
1	В	279	VAL	3.3
1	A	212	GLU	2.5
1	D	160	GLN	2.4
1	A	278	GLU	2.3

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 monosaccharides 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.

