



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:41 AM EDT

PDB ID : 3VOQ / pdb_00003voq
Title : Crystal structure of the pleckstrin homology domain of human Sin1, a TORC2 subunit
Authors : Pan, D.; Matsuura, Y.
Deposited on : 2012-01-31
Resolution : 2.00 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

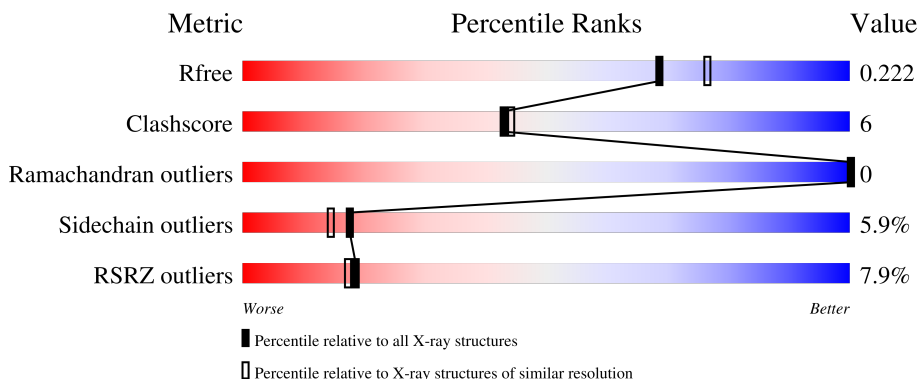
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

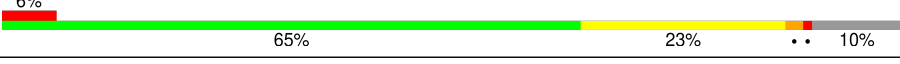
The reported resolution of this entry is 2.00 Å.

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	125	
1	B	125	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1930 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 Target of rapamycin complex 2 subunit MAPKAP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	0	0
			920	588	152	175	5			
1	B	113	Total	C	N	O	S	0	0	0
			885	561	147	172	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	369	GLY	-	expression tag	UNP Q9BPZ7
A	370	ALA	-	expression tag	UNP Q9BPZ7
A	371	MET	-	expression tag	UNP Q9BPZ7
B	369	GLY	-	expression tag	UNP Q9BPZ7
B	370	ALA	-	expression tag	UNP Q9BPZ7
B	371	MET	-	expression tag	UNP Q9BPZ7

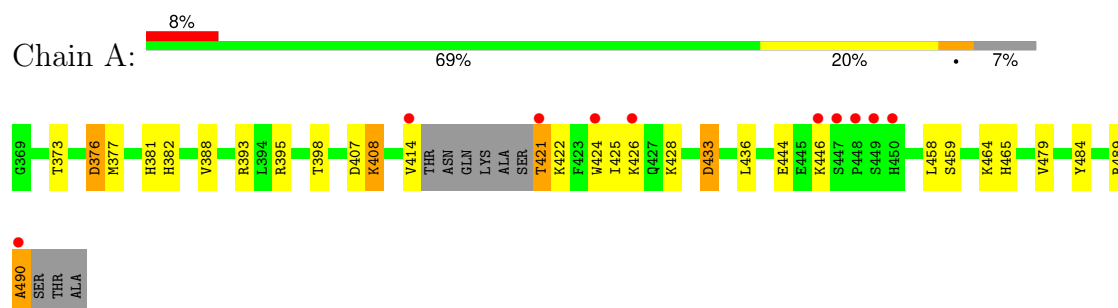
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	60	Total	O	0	0
			60	60		
2	B	65	Total	O	0	0
			65	65		

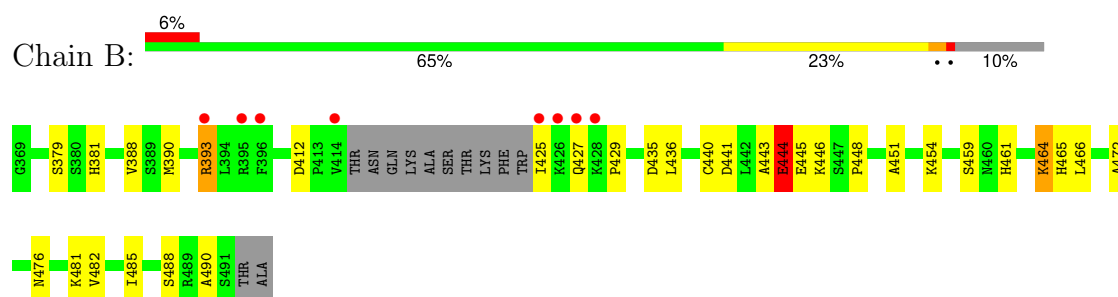
3 Residue-property plots [i](#)

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: Target of rapamycin complex 2 subunit MAPKAP1



- Molecule 1: Target of rapamycin complex 2 subunit MAPKAP1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.29Å 79.29Å 123.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.53 – 2.00 41.53 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.53-2.00) 99.9 (41.53-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.193 , 0.224 0.192 , 0.222	Depositor DCC
R_{free} test set	1371 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1930	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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 ⓘ

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	1.83	14/939 (1.5%)	1.40	6/1270 (0.5%)
1	B	1.82	14/901 (1.6%)	1.47	8/1218 (0.7%)
All	All	1.82	28/1840 (1.5%)	1.43	14/2488 (0.6%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	HIS	ND1-CE1	7.61	1.40	1.32
1	B	381	HIS	CG-CD2	7.14	1.43	1.35
1	B	461	HIS	CG-CD2	7.01	1.43	1.35
1	A	382	HIS	CG-CD2	6.76	1.43	1.35
1	B	465	HIS	CE1-NE2	6.73	1.39	1.32
1	B	436	LEU	N-CA	6.55	1.54	1.46
1	B	379	SER	CB-OG	-6.54	1.29	1.42
1	A	428	LYS	CA-C	6.32	1.61	1.53
1	A	382	HIS	ND1-CE1	6.25	1.38	1.32
1	B	465	HIS	CG-CD2	6.06	1.42	1.35
1	B	441	ASP	CA-C	-6.05	1.45	1.52
1	A	479	VAL	CA-C	6.04	1.60	1.52
1	A	484	TYR	N-CA	5.91	1.53	1.46
1	B	461	HIS	ND1-CE1	5.79	1.38	1.32
1	A	465	HIS	ND1-CE1	5.70	1.38	1.32
1	B	459	SER	C-O	5.67	1.30	1.23
1	A	388	VAL	CA-C	5.67	1.58	1.52
1	A	381	HIS	CG-ND1	-5.66	1.32	1.38
1	A	381	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	407	ASP	N-CA	5.55	1.53	1.46
1	A	422	LYS	CA-C	5.49	1.59	1.52
1	A	490	ALA	N-CA	5.44	1.56	1.46
1	B	490	ALA	N-CA	5.41	1.52	1.45
1	B	485	ILE	CA-CB	5.35	1.61	1.54
1	A	433	ASP	CB-CG	5.28	1.65	1.52
1	B	481	LYS	N-CA	5.19	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	436	LEU	N-CA	5.18	1.52	1.46
1	B	435	ASP	CA-C	5.16	1.60	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	ARG	O-C-N	-6.88	114.41	122.87
1	B	388	VAL	CA-C-N	-6.51	114.01	123.00
1	B	388	VAL	C-N-CA	-6.51	114.01	123.00
1	B	464	LYS	CB-CA-C	-6.08	98.76	109.71
1	A	376	ASP	CB-CA-C	-5.71	101.32	110.79
1	B	379	SER	N-CA-CB	-5.69	101.76	110.12
1	A	407	ASP	CB-CA-C	-5.59	100.47	110.70
1	A	489	ARG	CA-C-N	-5.44	111.91	121.70
1	A	489	ARG	C-N-CA	-5.44	111.91	121.70
1	B	444	GLU	CB-CG-CD	5.35	121.69	112.60
1	A	395	ARG	CA-CB-CG	-5.34	103.41	114.10
1	B	443	ALA	N-CA-C	-5.34	106.83	113.55
1	B	381	HIS	N-CA-C	5.09	119.49	113.28
1	B	472	ALA	N-CA-C	5.09	117.72	111.82

There are no chirality outliers.

There are no planarity outliers.

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	920	0	902	11	0
1	B	885	0	868	13	0
2	A	60	0	0	4	0
2	B	65	0	0	3	0
All	All	1930	0	1770	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 6.

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:433:ASP:HB2	2:A:543:HOH:O	1.68	0.93
1:B:393:ARG:HH12	1:B:425:ILE:HD13	1.37	0.89
1:A:424:TRP:HH2	2:A:541:HOH:O	1.60	0.85
1:B:390:MET:HE3	1:B:466:LEU:HD22	1.69	0.73
1:B:488:SER:HB2	2:B:520:HOH:O	1.90	0.72
1:A:490:ALA:C	2:A:517:HOH:O	2.33	0.71
1:A:398:THR:HG22	1:B:444:GLU:HG2	1.76	0.67
1:B:476:ASN:HB2	2:B:515:HOH:O	2.04	0.58
1:A:424:TRP:CZ3	1:A:426:LYS:HA	2.45	0.51
1:B:393:ARG:NH1	1:B:425:ILE:HD13	2.17	0.49
1:B:412:ASP:OD2	1:B:429:PRO:HB3	2.14	0.48
1:B:445:GLU:HG3	1:B:451:ALA:HB2	1.96	0.48
1:B:446:LYS:NZ	2:B:546:HOH:O	2.47	0.48
1:A:408:LYS:HE3	1:A:408:LYS:HB3	1.53	0.47
1:A:421:THR:HA	1:A:424:TRP:HB2	1.96	0.47
1:A:373:THR:HG22	1:A:377:MET:HE3	1.97	0.46
1:A:425:ILE:HD11	1:B:454:LYS:HD2	2.00	0.43
1:A:446:LYS:HE3	1:A:446:LYS:HB3	1.89	0.43
1:B:440:CYS:HB2	1:B:482:VAL:HG11	2.01	0.41
1:B:390:MET:CE	1:B:466:LEU:HD22	2.43	0.41
1:A:459:SER:HB3	1:A:464:LYS:HE3	2.02	0.41
2:A:528:HOH:O	1:B:454:LYS:HE3	2.20	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	Percentiles	
1	A	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
1	B	109/125 (87%)	105 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	221/250 (88%)	209 (95%)	12 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	103/112 (92%)	96 (93%)	7 (7%)	14	11
1	B	100/112 (89%)	95 (95%)	5 (5%)	22	20
All	All	203/224 (91%)	191 (94%)	12 (6%)	18	14

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

Mol	Chain	Res	Type
1	A	376	ASP
1	A	393	ARG
1	A	408	LYS
1	A	414	VAL
1	A	421	THR
1	A	444	GLU
1	A	458	LEU
1	B	393	ARG
1	B	427	GLN
1	B	444	GLU
1	B	448	PRO
1	B	464	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 oligosaccharides 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, 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	116/125 (92%)	0.28	10 (8%) 16 15	18, 32, 70, 92	0
1	B	113/125 (90%)	-0.00	8 (7%) 22 20	18, 29, 65, 87	0
All	All	229/250 (91%)	0.14	18 (7%) 18 17	18, 30, 68, 92	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	THR	6.3
1	B	425	ILE	5.7
1	A	490	ALA	5.3
1	A	424	TRP	3.9
1	A	414	VAL	3.5
1	B	396	PHE	3.4
1	B	426	LYS	3.2
1	A	448	PRO	3.1
1	A	450	HIS	3.0
1	B	427	GLN	2.7
1	A	446	LYS	2.7
1	B	395	ARG	2.7
1	B	393	ARG	2.7
1	B	414	VAL	2.3
1	B	428	LYS	2.3
1	A	447	SER	2.2
1	A	426	LYS	2.1
1	A	449	SER	2.0

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 oligosaccharides 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.