



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:47 PM GMT

PDB ID : 1CKB  
Title : STRUCTURAL BASIS FOR THE SPECIFIC INTERACTION OF LYSINE-CONTAINING PROLINE-RICH PEPTIDES WITH THE N-TERMINAL SH3 DOMAIN OF C-CRK  
Authors : Wu, X.; Kuriyan, J.  
Deposited on : 1995-01-24  
Resolution : 1.90 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

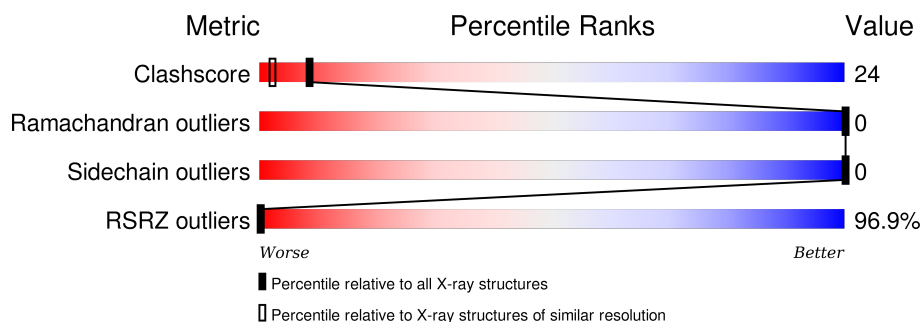
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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  $\geq 3$ , 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	57	<div> <div>96%</div> <div> <div>58%</div> <div>42%</div> </div> </div>
2	B	10	<div> <div>80%</div> <div> <div>50%</div> <div>30%</div> <div>20%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 741 atoms, of which 136 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 C-CRK N-TERMINAL SH3 DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	57	Total	C	N	O	S	0	0	0
			480	307	80	92	1			

- Molecule 2 is a protein called SOS PEPTIDE (PRO-PRO-PRO-VAL-PRO-PRO-ARG-ARG-ARG-ARG).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			57	39	11	7			

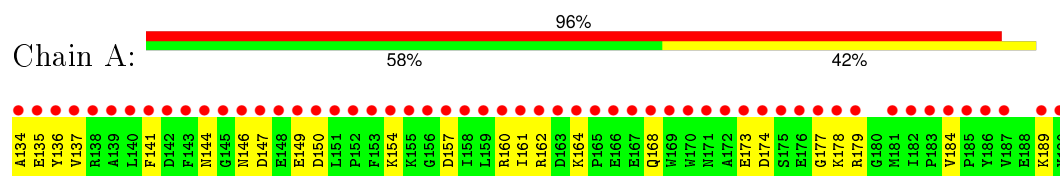
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	66	Total	H	O	0	0
			198	132	66		
3	B	2	Total	H	O	0	0
			6	4	2		

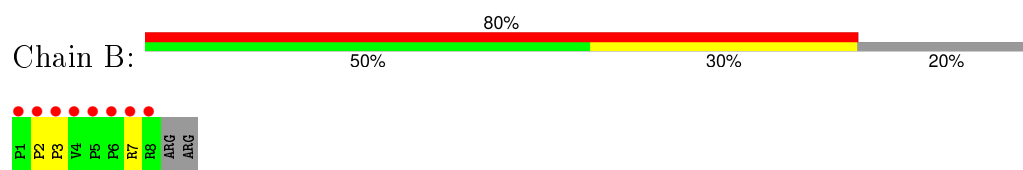
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: C-CRK N-TERMINAL SH3 DOMAIN



- Molecule 2: SOS PEPTIDE (PRO-PRO-PRO-VAL-PRO-PRO-ARG-ARG-ARG-ARG)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.40 Å 47.40 Å 29.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.90 25.05 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-1.90) 95.7 (25.05-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 1.90 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.183 , (Not available) 0.477 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	12.1	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 124.4	EDS
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 5107 reflections	Xtriage
$F_o, F_c$ correlation	0.54	EDS
Total number of atoms	741	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.59	0/493	0.70	0/665
2	B	0.48	0/61	0.88	0/86
All	All	0.58	0/554	0.72	0/751

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

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	480	0	450	24	7
2	B	57	0	61	3	0
3	A	66	132	0	21	6
3	B	2	4	0	1	0
All	All	605	136	511	25	8

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 24.

All (25) 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)
2:B:3:PRO:HG2	3:B:303:HOH:O	1.47	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:HG2	3:A:302:HOH:O	1.60	1.01
1:A:147:ASP:HB3	3:A:308:HOH:O	1.60	1.00
1:A:160:ARG:HG2	3:A:343:HOH:O	1.63	0.98
1:A:149:GLU:O	3:A:332:HOH:O	1.82	0.97
1:A:173:GLU:OE1	3:A:360:HOH:O	1.85	0.94
1:A:135:GLU:OE1	3:A:363:HOH:O	1.85	0.92
1:A:174:ASP:O	3:A:362:HOH:O	1.95	0.85
1:A:184:VAL:HG11	3:A:309:HOH:O	1.85	0.75
1:A:189:LYS:HE2	3:A:325:HOH:O	1.91	0.71
1:A:154:LYS:HE2	3:A:349:HOH:O	1.92	0.68
1:A:160:ARG:CG	3:A:343:HOH:O	2.35	0.61
1:A:144:ASN:OD1	3:A:351:HOH:O	2.17	0.60
1:A:137:VAL:HG12	3:A:322:HOH:O	2.01	0.60
1:A:136:TYR:HB2	3:A:327:HOH:O	2.04	0.58
1:A:178:LYS:HG2	3:A:355:HOH:O	2.04	0.57
1:A:150:ASP:OD1	2:B:7:ARG:NH2	2.38	0.56
1:A:146:ASN:ND2	3:A:319:HOH:O	2.41	0.53
1:A:189:LYS:HA	3:A:305:HOH:O	2.12	0.48
1:A:136:TYR:O	3:A:305:HOH:O	2.20	0.48
1:A:161:ILE:HG22	3:A:358:HOH:O	2.14	0.47
1:A:168:GLN:HB2	3:A:345:HOH:O	2.13	0.47
1:A:134:ALA:HB3	1:A:136:TYR:CE2	2.50	0.47
1:A:177:GLY:N	3:A:362:HOH:O	2.53	0.41
1:A:141:PHE:CE1	2:B:2:PRO:HD3	2.56	0.41

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:O	3:A:346:HOH:H2[4_4104]	0.96	0.64
1:A:154:LYS:CG	1:A:162:ARG:NH2[3_1065]	1.78	0.42
1:A:161:ILE:O	3:A:324:HOH:H1[4_4104]	1.22	0.38
1:A:162:ARG:O	3:A:346:HOH:O[4_4104]	1.87	0.33
1:A:164:LYS:O	3:A:304:HOH:H2[3_1055]	1.34	0.26
1:A:157:ASP:OD2	1:A:179:ARG:NH2[3_1065]	1.98	0.22
1:A:161:ILE:O	3:A:324:HOH:O[4_4104]	2.12	0.08
3:A:324:HOH:O	3:A:358:HOH:H2[3_1065]	1.55	0.05

## 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	55/57 (96%)	55 (100%)	0	0	100	100
2	B	6/10 (60%)	6 (100%)	0	0	100	100
All	All	61/67 (91%)	61 (100%)	0	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	50/50 (100%)	50 (100%)	0	100	100
2	B	7/10 (70%)	7 (100%)	0	100	100
All	All	57/60 (95%)	57 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN

### 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 carbohydrates 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	57/57 (100%)	4.64	55 (96%) <b>0</b> <b>0</b>	4, 9, 23, 31	0
2	B	8/10 (80%)	4.43	8 (100%) <b>0</b> <b>0</b>	11, 13, 31, 37	0
All	All	65/67 (97%)	4.61	63 (96%) <b>0</b> <b>0</b>	4, 10, 24, 37	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	ILE	10.0
1	A	190	TYR	9.6
1	A	152	PRO	8.1
1	A	145	GLY	8.1
1	A	143	PHE	7.5
1	A	149	GLU	6.7
1	A	141	PHE	6.5
1	A	136	TYR	6.4
2	B	6	PRO	6.2
1	A	185	PRO	6.1
1	A	184	VAL	6.0
1	A	182	ILE	6.0
1	A	159	LEU	5.9
1	A	140	LEU	5.8
1	A	169	TRP	5.8
2	B	2	PRO	5.7
1	A	165	PRO	5.7
1	A	158	ILE	5.6
1	A	181	MET	5.6
2	B	7	ARG	5.5
1	A	187	VAL	5.3
1	A	177	GLY	5.2
2	B	1	PRO	5.2
1	A	189	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	134	ALA	5.1
1	A	175	SER	5.1
1	A	154	LYS	5.0
1	A	144	ASN	4.9
1	A	186	TYR	4.7
1	A	146	ASN	4.6
1	A	137	VAL	4.5
1	A	148	GLU	4.4
1	A	163	ASP	4.4
1	A	170	TRP	4.4
1	A	157	ASP	4.1
1	A	176	GLU	4.1
1	A	156	GLY	3.9
1	A	171	ASN	3.9
1	A	167	GLU	3.9
1	A	142	ASP	3.8
1	A	172	ALA	3.8
1	A	151	LEU	3.7
1	A	147	ASP	3.7
2	B	8	ARG	3.7
1	A	179	ARG	3.6
2	B	5	PRO	3.6
1	A	178	LYS	3.5
1	A	174	ASP	3.5
1	A	173	GLU	3.5
1	A	166	GLU	3.4
1	A	183	PRO	3.4
1	A	153	PHE	3.4
1	A	139	ALA	3.3
1	A	138	ARG	3.3
1	A	155	LYS	3.2
2	B	3	PRO	2.8
2	B	4	VAL	2.7
1	A	150	ASP	2.6
1	A	162	ARG	2.4
1	A	168	GLN	2.3
1	A	164	LYS	2.3
1	A	160	ARG	2.3
1	A	135	GLU	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 carbohydrates 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.