

# wwPDB X-ray Structure Validation Summary Report (i)

#### Jan 27, 2024 - 06:31 PM EST

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 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:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

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		Percentile Ranks	Value
Clashscore			24
Ramachandran outliers			0
Sidechain outliers			0
	Worse		Better
	Percentile relative to all X-ray	y structures	
	Percentile relative to X-ray st	tructures of similar resolution	

Metric	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 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%

Mol	Chain	Length	Quality of chain				
1	А	57	58% 42%				
2	В	10	50%	30%	20%		



# 2 Entry composition (i)

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	А	57	Total 480	C 307	N 80	O 92	S 1	0	0	0

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

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

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	66	Total         H         O           198         132         66	0	0
3	В	2	$\begin{array}{cccc} \text{Total} & \text{H} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0



# 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. 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. 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

Chain A:		58%	4	12%	l
A134 E135 V137 V137 F141 F141 N144 0145	N146 D147 E148 E149 D150 K154 K154 D157	R160 1161 R162 D163 R164 R164 R164 E173 D174 D174	K178 R179 V184 V184 K189 Y190		
• Molecule 2	2: SOS PEPT	IDE (PRO-PRO-	-PRO-VAL-PRO-	PRO-ARG-AR	G-ARG-ARG)
Chain B:	5(	0%	30%	20%	I



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants	47.40Å 47.40Å 29.50Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	6.00 - 1.90	Depositor
Resolution (A)	25.05 - 1.90	EDS
% Data completeness	(Not available) $(6.00-1.90)$	Depositor
(in resolution range)	$95.7\ (25.05-1.90)$	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.13 (at 1.90 \text{\AA})$	Xtriage
Refinement program	X-PLOR	Depositor
P. P.	0.183 , (Not available)	Depositor
$R, R_{free}$	0.491 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	12.1	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.41 , $124.4$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.54	EDS
Total number of atoms	741	wwPDB-VP
Average B, all atoms $(Å^2)$	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>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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			lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.59	0/493	0.70	0/665	
2	В	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 (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	А	480	0	450	24	7
2	В	57	0	61	3	0
3	А	66	132	0	21	6
3	В	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.

The worst 5 of 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

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The worst 5 of 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

# 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	ntiles
1	А	55/57~(96%)	55 (100%)	0	0	100	100
2	В	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 (i)

In the following table, the Percentiles column shows the percent side chain 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.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	50/50~(100%)	50 (100%)	0	100	100
2	В	7/10 (70%)	7 (100%)	0	100	100
All	All	57/60~(95%)	57 (100%)	0	100	100

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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

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

Mol	Chain	Res	Type
1	А	146	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 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

