

wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 10:57 pm BST

PDB ID : 6QBN

Title: structure of the core domaine of Knr4, an intrinsically disordered protein from

Saccharomyces cerevisiae - mutant S200D

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D.

Deposited on : 2018-12-21

Resolution : 2.40 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 following versions of software and data (see references (1)) were used in the production of this report:

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

EDS: 2.11

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

Refmac: 5.8.0158

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

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

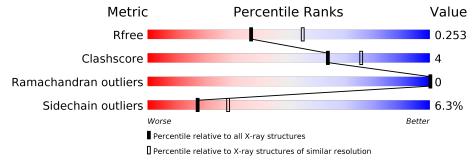
Validation Pipeline (wwPDB-VP) : 2.11

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 2.40 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 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	A	275	67%	10%		21%				
1	В	275	69%	9%		21%				



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3458 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 Cell wall assembly regulator SMI1.

\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	216	Total	С	N	О	S	0	0	0
1	Λ	210	1716	1100	285	327	4	0	U	0
1	B	216	Total	С	N	О	S	0	0	0
1	D	210	1737	1112	298	324	3		U	U

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	GLY	-	expression tag	UNP P32566
A	74	PRO	-	expression tag	UNP P32566
A	75	LEU	-	expression tag	UNP P32566
A	76	GLY	_	expression tag	UNP P32566
A	77	SER	-	expression tag	UNP P32566
A	78	HIS	-	expression tag	UNP P32566
A	79	MET	-	expression tag	UNP P32566
A	200	ASP	SER	engineered mutation	UNP P32566
A	341	LEU	-	expression tag	UNP P32566
A	342	GLU	_	expression tag	UNP P32566
A	343	ARG	-	expression tag	UNP P32566
A	344	PRO	-	expression tag	UNP P32566
A	345	HIS	-	expression tag	UNP P32566
A	346	ARG	-	expression tag	UNP P32566
A	347	ASP	-	expression tag	UNP P32566
В	73	GLY	-	expression tag	UNP P32566
В	74	PRO	_	expression tag	UNP P32566
В	75	LEU	_	expression tag	UNP P32566
В	76	GLY	-	expression tag	UNP P32566
В	77	SER	-	expression tag	UNP P32566
В	78	HIS	-	expression tag	UNP P32566
В	79	MET	-	expression tag	UNP P32566
В	200	ASP	SER	engineered mutation	UNP P32566
В	341	LEU		expression tag	UNP P32566
В	342	GLU	_	expression tag	UNP P32566

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Chain	Residue	Modelled	Actual Comment		Reference
В	343	ARG	_	expression tag	UNP P32566
В	344	PRO	-	expression tag	UNP P32566
В	345	HIS	_	expression tag	UNP P32566
В	346	ARG	-	expression tag	UNP P32566
В	347	ASP	_	expression tag	UNP P32566

• Molecule 2 is water.

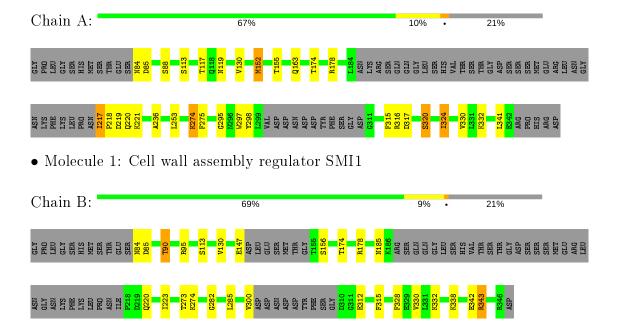
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	5	Total O 5 5	0	0



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. 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: Cell wall assembly regulator SMI1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62	Depositor
Cell constants	103.11Å 103.11Å 93.39Å	Domositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.18 - 2.40	Depositor
Resolution (A)	45.13 - 2.40	EDS
% Data completeness	95.3 (45.18-2.40)	Depositor
(in resolution range)	95.3 (45.13-2.40)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	1.55 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
D D.	0.180 , 0.217	Depositor
R, R_{free}	0.222 , 0.253	DCC
R_{free} test set	1080 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 25.9	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3458	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.26% 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		
		RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.73	0/1764	0.77	0/2405	
1	В	0.84	0/1786	0.79	0/2431	
All	All	0.79	0/3550	0.78	0/4836	

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	1716	0	1616	16	0
1	В	1737	0	1650	12	0
2	В	5	0	0	0	0
All	All	3458	0	3266	28	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 4.

The worst 5 of 28 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1			$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:298:TYR:CD2	1:A:324:ILE:HD11	2.23	0.73

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Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:A:298:TYR:HD2	1:A:324:ILE:HD11	1.56	0.70
1:B:338:LYS:O	1:B:342:GLU:HG3	1.93	0.68
1:B:174:THR:O	1:B:178:ARG:HG3	1.95	0.66
1:B:90:THR:HG22	1:B:282:GLY:CA	2.28	0.63

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	ntiles
1	A	210/275~(76%)	204 (97%)	6 (3%)	0	100	100
1	В	208/275~(76%)	206 (99%)	2 (1%)	0	100	100
All	All	418/550 (76%)	410 (98%)	8 (2%)	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 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	$182/239 \ (76\%)$	168 (92%)	14 (8%)	13 20
1	В	185/239 (77%)	176 (95%)	9 (5%)	25 40
All	All	367/478 (77%)	344 (94%)	23 (6%)	18 28



5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LYS
1	A	324	ILE
1	В	185	ASN
1	A	320	SER
1	A	341	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	84	ASN
1	A	119	ASN
1	A	169	GLN
1	В	84	ASN
1	В	96	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 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 (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.

