



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:54 PM GMT

PDB ID : 4GKQ
Title : Structure of the neck and C-terminal motor homology domain of ViK1 from *Candida glabrata*
Authors : Duan, D.; Allingham, J.S.
Deposited on : 2012-08-13
Resolution : 2.99 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

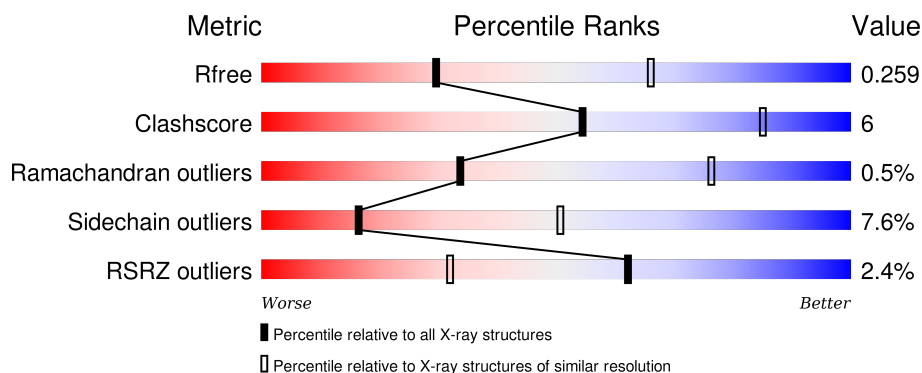
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

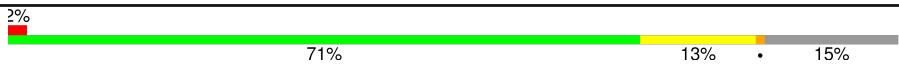
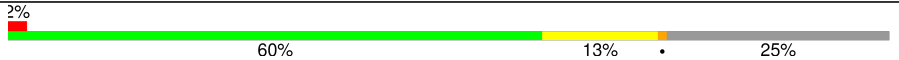
The reported resolution of this entry is 2.99 Å.

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	286	
1	B	286	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3324 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 SPINDLE POLE BODY-ASSOCIATED PROTEIN VIK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1752	1144	285	319	4			
1	B	214	Total	C	N	O	S	0	0	0
			1571	1037	247	284	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299	GLY	-	EXPRESSION TAG	UNP Q6FSG8
A	300	HIS	-	EXPRESSION TAG	UNP Q6FSG8
A	301	MET	-	EXPRESSION TAG	UNP Q6FSG8
B	299	GLY	-	EXPRESSION TAG	UNP Q6FSG8
B	300	HIS	-	EXPRESSION TAG	UNP Q6FSG8
B	301	MET	-	EXPRESSION TAG	UNP Q6FSG8

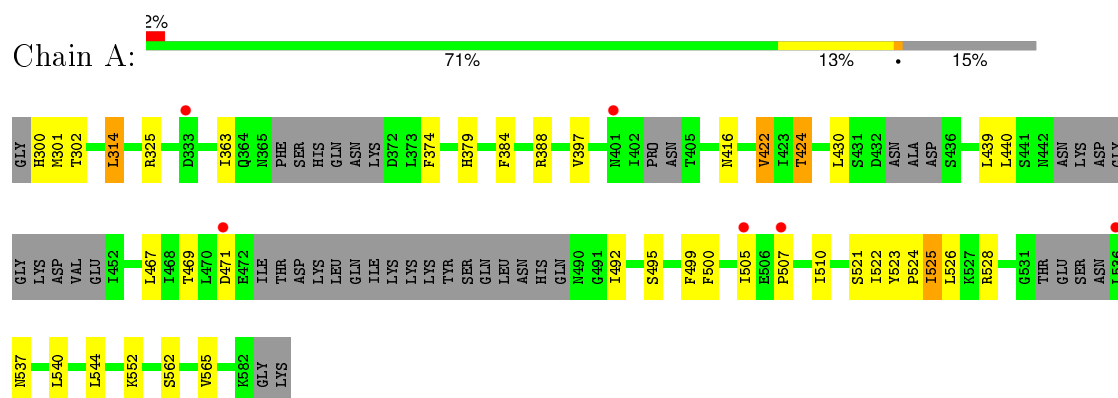
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		

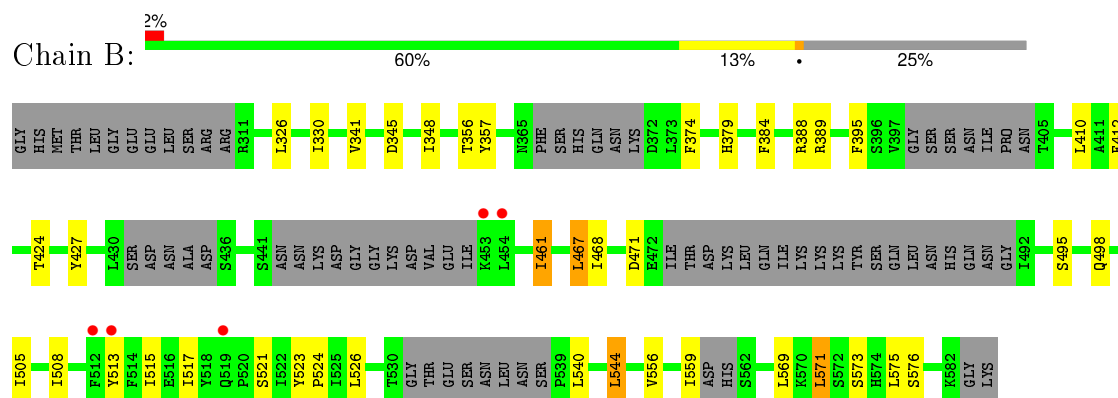
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: SPINDLE POLE BODY-ASSOCIATED PROTEIN VIK1



• Molecule 1: SPINDLE POLE BODY-ASSOCIATED PROTEIN VIK1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	197.00 Å 197.00 Å 50.18 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.80 – 2.99 19.80 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.80-2.99) 99.2 (19.80-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.98 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.214 , 0.259 0.213 , 0.259	Depositor DCC
R_{free} test set	1444 reflections (11.06%)	DCC
Wilson B-factor (Å ²)	108.6	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 93.0	EDS
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 14501 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3324	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.40	0/1782	0.56	1/2426 (0.0%)
1	B	0.40	0/1598	0.58	0/2172
All	All	0.40	0/3380	0.57	1/4598 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	LEU	CA-CB-CG	5.74	128.49	115.30

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	1752	0	1543	17	0
1	B	1571	0	1401	23	0
2	A	1	0	0	0	0
All	All	3324	0	2944	40	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 (40) 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:B:424:THR:HB	1:B:467:LEU:HD11	1.45	0.98
1:B:424:THR:HB	1:B:467:LEU:CD1	2.07	0.85
1:B:424:THR:OG1	1:B:498:GLN:HB2	1.86	0.75
1:B:348:ILE:HD11	1:B:569:LEU:HD21	1.75	0.68
1:B:374:PHE:HZ	1:B:556:VAL:HG21	1.64	0.62
1:A:422:VAL:HG13	1:A:500:PHE:HB2	1.82	0.62
1:B:427:TYR:CD1	1:B:495:SER:HB3	2.36	0.60
1:B:374:PHE:CZ	1:B:556:VAL:HG21	2.37	0.59
1:B:461:ILE:HG23	1:B:513:TYR:OH	2.03	0.58
1:A:424:THR:OG1	1:A:467:LEU:HD21	2.03	0.57
1:A:525:ILE:HG23	1:A:528:ARG:HH21	1.71	0.56
1:A:537:ASN:OD1	1:A:537:ASN:N	2.37	0.56
1:B:341:VAL:HA	1:B:348:ILE:HG22	1.87	0.56
1:A:325:ARG:NH1	1:A:552:LYS:HD3	2.20	0.56
1:B:384:PHE:O	1:B:388:ARG:HG3	2.07	0.55
1:B:521:SER:O	1:B:524:PRO:HD2	2.07	0.53
1:B:326:LEU:HD11	1:B:576:SER:HB3	1.92	0.51
1:B:523:TYR:HB2	1:B:524:PRO:HD3	1.92	0.51
1:B:395:PHE:CZ	1:B:515:ILE:HD12	2.48	0.48
1:A:522:ILE:O	1:A:522:ILE:HG22	2.12	0.48
1:B:389:ARG:NH2	1:B:508:ILE:HG13	2.29	0.48
1:B:379:HIS:HD2	1:B:412:PHE:HZ	1.61	0.48
1:A:469:THR:HG22	1:A:471:ASP:H	1.79	0.47
1:A:374:PHE:O	1:A:379:HIS:HB2	2.14	0.47
1:B:526:LEU:HD23	1:B:571:LEU:HD11	1.97	0.46
1:A:300:HIS:HA	1:A:301:MET:HA	1.69	0.46
1:A:499:PHE:HB2	1:A:510:ILE:HB	1.98	0.46
1:A:523:TYR:N	1:A:524:PRO:HD2	2.31	0.46
1:B:326:LEU:HD11	1:B:576:SER:CB	2.47	0.44
1:B:379:HIS:HD2	1:B:412:PHE:CZ	2.36	0.43
1:B:357:TYR:HD2	1:B:573:SER:HG	1.64	0.43
1:A:562:SER:O	1:A:565:VAL:HG23	2.18	0.43
1:A:384:PHE:CZ	1:A:388:ARG:HD2	2.53	0.43
1:B:517:ILE:HD12	1:B:526:LEU:HD22	2.02	0.42
1:A:492:ILE:HG12	1:A:540:LEU:HD21	2.02	0.41
1:A:505:ILE:O	1:A:507:PRO:HD3	2.20	0.41
1:A:430:LEU:HD23	1:A:540:LEU:HD23	2.03	0.40
1:B:330:ILE:HD13	1:B:559:ILE:HB	2.03	0.40
1:A:416:ASN:HD22	1:A:416:ASN:HA	1.72	0.40
1:B:544:LEU:HD12	1:B:544:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

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	228/286 (80%)	213 (93%)	15 (7%)	0	100	100
1	B	198/286 (69%)	179 (90%)	17 (9%)	2 (1%)	19	61
All	All	426/572 (74%)	392 (92%)	32 (8%)	2 (0%)	34	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	471	ASP
1	B	505	ILE

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	158/269 (59%)	145 (92%)	13 (8%)	14	46
1	B	145/269 (54%)	135 (93%)	10 (7%)	19	56
All	All	303/538 (56%)	280 (92%)	23 (8%)	16	51

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	THR
1	A	314	LEU
1	A	363	ILE
1	A	397	VAL

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Mol	Chain	Res	Type
1	A	422	VAL
1	A	424	THR
1	A	439	LEU
1	A	440	LEU
1	A	495	SER
1	A	521	SER
1	A	525	ILE
1	A	526	LEU
1	A	544	LEU
1	B	345	ASP
1	B	356	THR
1	B	410	LEU
1	B	461	ILE
1	B	467	LEU
1	B	468	ILE
1	B	540	LEU
1	B	544	LEU
1	B	571	LEU
1	B	575	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	HIS
1	A	416	ASN
1	B	379	HIS
1	B	580	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 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](#)

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	242/286 (84%)	-0.29	6 (2%) 61 30	74, 109, 159, 192	0
1	B	214/286 (74%)	-0.18	5 (2%) 64 33	78, 119, 164, 180	0
All	All	456/572 (79%)	-0.24	11 (2%) 62 32	74, 114, 164, 192	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	453	LYS	3.5
1	A	333	ASP	3.0
1	A	536	LEU	2.9
1	B	454	LEU	2.7
1	A	507	PRO	2.5
1	A	471	ASP	2.4
1	A	505	ILE	2.2
1	B	512	PHE	2.2
1	B	513	TYR	2.0
1	A	401	ASN	2.0
1	B	519	GLN	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.