wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2EQX
Title	:	Solution structure of the BACK domain of Kelch repeat and BTB domain-containing protein 4
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This is a wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

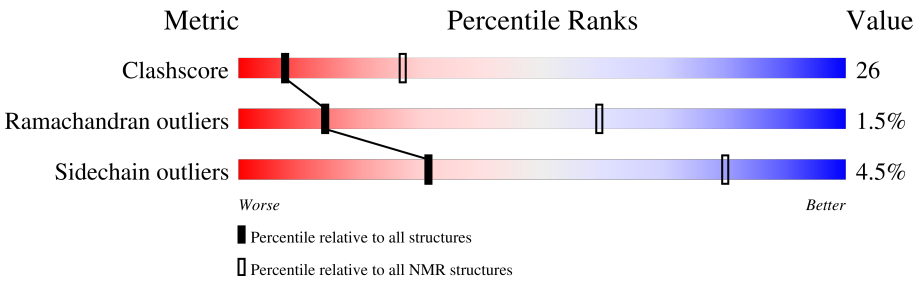
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	105	50% 38% 12%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:159-A:250 (92)	0.17	6

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 5, 6, 8, 9, 13, 14, 15, 16, 17, 18, 20
2	4, 7, 11, 12, 19
Single-model clusters	10

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1602 atoms, of which 783 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Kelch repeat and BTB domain-containing protein 4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	105	1602	507	783	146	162	4	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	GLY	-	expression tag	UNP Q9NVX7
A	152	SER	-	expression tag	UNP Q9NVX7
A	153	SER	-	expression tag	UNP Q9NVX7
A	154	GLY	-	expression tag	UNP Q9NVX7
A	155	SER	-	expression tag	UNP Q9NVX7
A	156	SER	-	expression tag	UNP Q9NVX7
A	157	GLY	-	expression tag	UNP Q9NVX7

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Kelch repeat and BTB domain-containing protein 4

Chain A: 50% 38% 12%

G151 S152 S153 G154 S155 S156 G157 V158 Q159 V160 G161 N162 C163 L164 Q165 V166 M167 W168 L169 A170 D171 R172 H173 L178 Y179 L190 L193 Q194 E197 E198 F199 L200 H201 L202 L206 P216 C217 S218 Q219 N220 P221 I225 W228 I229 N232 K233 E234 E235 R236 E237 A238

F239 A240 S246 L247 K248 G251 E252 N253 V254 H255

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 6. Colouring as in section 4.1 above.

• Molecule 1: Kelch repeat and BTB domain-containing protein 4

Chain A: 47% 36% 5% 12%

G151 S152 S153 G154 S155 S156 G157 V158 Q159 V160 G161 N162 C163 L164 Q165 V166 M167 W168 L169 H173 S174 D175 L178 Y179 T180 H184 K187 Q194 E197 E198 F199 L200 H201 L202 D209 P216 C217 S218 Q219 N220 P221 A224 I225 W228 I229 N232 K233 E234 E235

R236 E237 A238 F239 A240 L247 K248 G251 E252 N253 V254 H255

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dyanamics, simulated annealing.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy, target function.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	738	714	714	37±5
All	All	14760	14280	14280	743

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 26.

5 of 179 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:225:ILE:CD1	1:A:247:LEU:HD12	0.87	1.99	8	17
1:A:164:LEU:HD22	1:A:202:LEU:HD11	0.84	1.49	16	16
1:A:164:LEU:HD12	1:A:198:GLU:OE1	0.84	1.71	6	1
1:A:204:HIS:CE1	1:A:239:PHE:CD1	0.79	2.70	14	2
1:A:204:HIS:CE1	1:A:239:PHE:CE1	0.79	2.71	14	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	92/105 (88%)	68±2 (74±3%)	23±2 (25±3%)	1±1 (2±1%)	14 59
All	All	1840/2100 (88%)	1359 (74%)	453 (25%)	28 (2%)	14 59

5 of 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	233	LYS	6
1	A	220	ASN	5
1	A	160	VAL	5
1	A	217	CYS	4
1	A	166	VAL	4

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	81/90 (90%)	77±1 (95±1%)	4±1 (5±1%)	31 80
All	All	1620/1800 (90%)	1547 (95%)	73 (5%)	31 80

5 of 19 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	194	GLN	16
1	A	162	ASN	13
1	A	248	LYS	5
1	A	230	ASN	5
1	A	209	ASP	4

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided