wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2E6I
Title	:	Solution structure of the BTK motif of tyrosine-protein kinase ITK from human
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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:

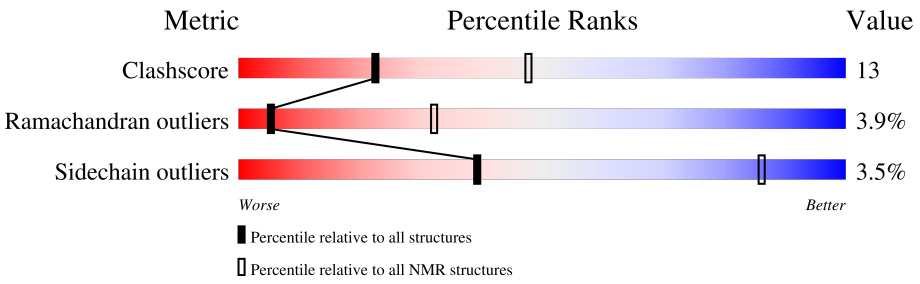
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	64	30% 12% 58%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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:12-A:20, A:24-A:41 (27)	0.22	11

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 3 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 980 atoms, of which 478 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	64	979	313	478	91	93	4	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q08881
A	2	SER	-	cloning artifact	UNP Q08881
A	3	SER	-	cloning artifact	UNP Q08881
A	4	GLY	-	cloning artifact	UNP Q08881
A	5	SER	-	cloning artifact	UNP Q08881
A	6	SER	-	cloning artifact	UNP Q08881
A	7	GLY	-	cloning artifact	UNP Q08881

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

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: Tyrosine-protein kinase ITK/TSK

Chain A: 30% 12% 58%

G1 S2 S3 G4 S5 S6 G7 N8 N9 S10 L11 H16 F19 W20 M21 D22 G23 K24 W25 L31 T36 G37 Y41 D42 P43 T44 K45 N46 A47 S48 K49 K50 P51 L52 P53 P54 T55 P56 E57 D58 N59 R60 R61 P62 L63 W64

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

The representative model is number 11. Colouring as in section 4.1 above.

- Molecule 1: Tyrosine-protein kinase ITK/TSK

Chain A: 23% 16% • 58%

G1 S2 S3 G4 S5 S6 G7 N8 N9 S10 L11 V12 P13 K14 Y15 H16 W20 M21 D22 G23 K24 W25 K33 L34 A35 T36 G37 C38 A39 Q40 Y41 D42 P43 T44 K45 N46 A47 S48 K49 K50 P51 L52 P53 P54 T55 P56 E57 D58 N59 R60 R61 P62 L63 W64

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

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

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	228	216	216	6±2
All	All	4580	4320	4320	112

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 13.

5 of 53 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:HIS:CD2	1:A:25:TRP:CH2	0.80	2.70	15	6
1:A:16:HIS:CD2	1:A:25:TRP:CZ2	0.78	2.72	14	11
1:A:31:LEU:HD12	1:A:31:LEU:O	0.74	1.82	3	2
1:A:12:VAL:HG23	1:A:41:TYR:CE2	0.63	2.27	3	1
1:A:12:VAL:HG11	1:A:40:GLN:OE1	0.63	1.93	7	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	27/64 (42%)	22±1 (82±4%)	4±1 (14±5%)	1±1 (4±3%)	5 32
All	All	540/1280 (42%)	441 (82%)	78 (14%)	21 (4%)	5 32

All 3 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	37	GLY	12
1	A	41	TYR	8
1	A	35	ALA	1

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	24/56 (43%)	23±1 (96±4%)	1±1 (4±4%)	39 86
All	All	480/1120 (43%)	463 (96%)	17 (4%)	39 86

5 of 7 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	19	PHE	5
1	A	31	LEU	4
1	A	41	TYR	3
1	A	33	LYS	2
1	A	20	TRP	1

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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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