Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2K79
Title	:	Solution Structure of the binary complex between the SH3 and SH2 domain of interleukin-2 tyrosine kinase
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Deposited on	:	2008-08-08

This is a Full wwPDB NMR Structure Validation 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 (1)) were used in the production of this report:

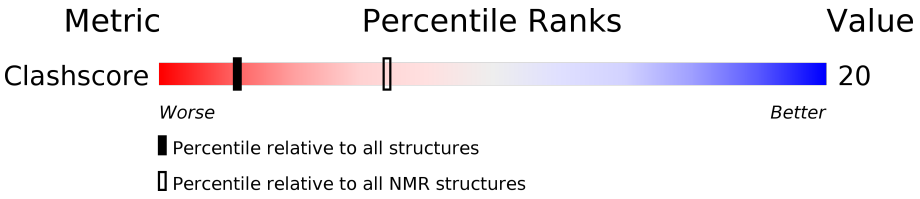
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

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	63	70% 30%
2	B	110	62% 36% .

2 Ensemble composition and analysis

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2749 atoms, of which 1345 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SH3 domain of Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	63	993	328	473	82	109	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	GLY	-	expression tag	UNP Q03526
A	170	SER	-	expression tag	UNP Q03526

- Molecule 2 is a protein called SH2 domain of Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	108	1756	565	872	150	166	3	0

There are 3 discrepancies between the modelled and reference sequences:

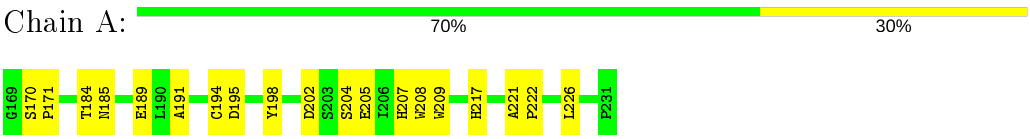
Chain	Residue	Modelled	Actual	Comment	Reference
B	230	GLY	-	expression tag	UNP Q03526
B	231	SER	-	expression tag	UNP Q03526
B	339	GLY	-	expression tag	UNP Q03526

4 Residue-property plots (i)

These plots are provided for all protein, RNA and DNA 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.

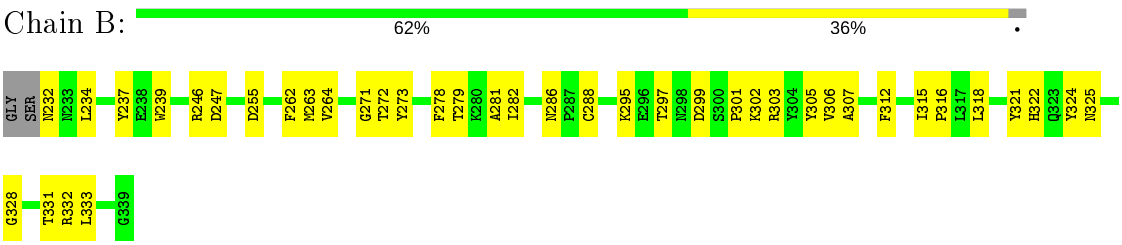
- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

Chain A:



- Molecule 2: SH2 domain of Tyrosine-protein kinase ITK/TSK

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the ? calculated structures, 1 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
xplor-nih	refinement	2.19

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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	520	473	470	20
2	B	884	872	870	39
All	All	1404	1345	1340	54

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 20.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:222:PRO:O	1:A:226:LEU:HD12	0.83	1.73
1:A:208:TRP:HE1	2:B:328:GLY:C	0.74	1.85
2:B:306:VAL:HG23	2:B:306:VAL:O	0.70	1.85
1:A:184:THR:OG1	1:A:191:ALA:N	0.56	2.38
2:B:278:PHE:CD1	2:B:279:THR:N	0.56	2.73
2:B:232:ASN:O	2:B:234:LEU:N	0.56	2.38
1:A:208:TRP:HE1	2:B:328:GLY:CA	0.56	2.13
1:A:170:SER:N	1:A:171:PRO:CD	0.54	2.70
1:A:205:GLU:OE1	1:A:207:HIS:NE2	0.53	2.42
2:B:306:VAL:CG2	2:B:306:VAL:O	0.52	2.55
2:B:331:THR:O	2:B:332:ARG:O	0.52	2.27
2:B:273:TYR:N	2:B:273:TYR:CD1	0.50	2.79
1:A:205:GLU:O	1:A:209:TRP:NE1	0.49	2.45
1:A:221:ALA:HB1	1:A:226:LEU:HD11	0.49	1.83

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:184:THR:CG2	1:A:185:ASN:N	0.49	2.75
2:B:315:ILE:N	2:B:316:PRO:HD2	0.49	2.22
1:A:194:CYS:SG	1:A:195:ASP:N	0.49	2.85
1:A:184:THR:HG22	1:A:185:ASN:N	0.49	2.23
2:B:301:PRO:O	2:B:302:LYS:O	0.48	2.31
2:B:263:MET:CG	2:B:264:VAL:N	0.48	2.76
2:B:282:ILE:HD12	2:B:288:CYS:SG	0.48	2.49
2:B:305:TYR:C	2:B:305:TYR:CD1	0.47	2.86
1:A:185:ASN:HD22	2:B:332:ARG:NH1	0.47	2.07
2:B:333:LEU:CD1	2:B:333:LEU:H	0.47	2.22
2:B:332:ARG:O	2:B:333:LEU:C	0.47	2.53
1:A:198:TYR:N	1:A:198:TYR:CD1	0.47	2.82
2:B:286:ASN:OD1	2:B:286:ASN:O	0.47	2.33
1:A:208:TRP:N	1:A:208:TRP:CD1	0.46	2.83
2:B:333:LEU:HD12	2:B:333:LEU:N	0.46	2.24
1:A:189:GLU:OE2	1:A:208:TRP:CH2	0.46	2.69
1:A:208:TRP:NE1	2:B:328:GLY:CA	0.45	2.79
2:B:324:TYR:O	2:B:325:ASN:C	0.45	2.54
2:B:281:ALA:O	2:B:282:ILE:O	0.45	2.35
2:B:297:THR:OG1	2:B:297:THR:O	0.45	2.34
2:B:262:PHE:CD1	2:B:262:PHE:C	0.44	2.91
2:B:306:VAL:O	2:B:307:ALA:HB2	0.44	2.12
2:B:299:ASP:C	2:B:301:PRO:O	0.44	2.56
1:A:202:ASP:OD1	1:A:204:SER:OG	0.43	2.35
2:B:255:ASP:O	2:B:255:ASP:OD1	0.43	2.36
2:B:295:LYS:O	2:B:303:ARG:O	0.43	2.37
2:B:325:ASN:N	2:B:325:ASN:ND2	0.42	2.67
2:B:271:GLY:O	2:B:272:THR:OG1	0.42	2.35
2:B:312:PHE:CZ	2:B:321:TYR:CD2	0.42	3.08
2:B:333:LEU:HD12	2:B:333:LEU:H	0.42	1.74
2:B:318:LEU:HD23	2:B:322:HIS:HD1	0.41	1.75
1:A:208:TRP:NE1	2:B:328:GLY:C	0.41	2.66
1:A:217:HIS:CD2	1:A:217:HIS:N	0.41	2.89
2:B:333:LEU:N	2:B:333:LEU:CD1	0.41	2.83
2:B:278:PHE:C	2:B:278:PHE:CD1	0.41	2.89
1:A:189:GLU:CD	1:A:208:TRP:CH2	0.40	2.94
2:B:237:TYR:CG	2:B:239:TRP:CZ2	0.40	3.08
2:B:246:ARG:CG	2:B:247:ASP:N	0.40	2.84
2:B:321:TYR:C	2:B:321:TYR:CD1	0.40	2.95
2:B:315:ILE:N	2:B:316:PRO:CD	0.40	2.85

6.3 Torsion angles

6.3.1 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 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	0	-	-	-	-
2	B	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

6.3.2 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 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	0	-	-	-
2	B	0	-	-	-
All	All	0	-	-	-

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

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided