



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2K79 / pdb_00002k79
BMRB ID : 15912
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

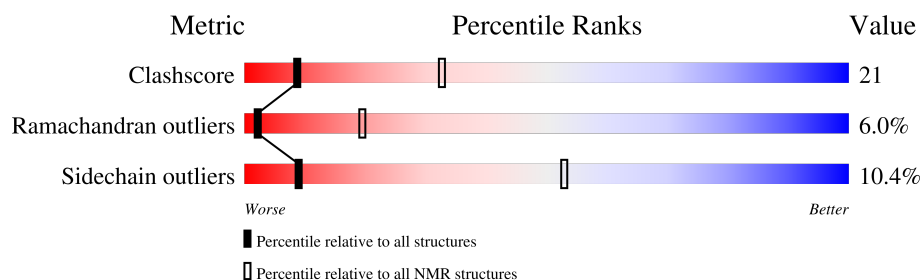
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	63	 63% 35% .
2	B	110	 55% 33% 10% ..

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
1	A	63	Total	C	H	N	O	S	0
			993	328	473	82	109	1	

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
2	B	108	Total	C	H	N	O	S	0
			1756	565	872	150	166	3	

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

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.

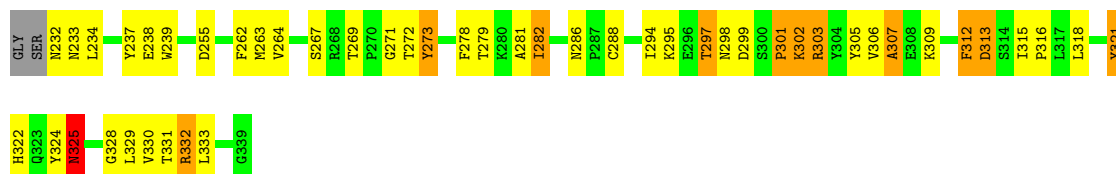
- Molecule 1: SH3 domain of Tyrosine-protein kinase ITK/TSK

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.

6 Model quality [i](#)

6.1 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 (average) 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	0.74	0/535 (0.0%)	1.01	0/729 (0.0%)
2	B	0.68	0/906 (0.0%)	0.95	1/1225 (0.1%)
All	All	0.70	0/1441 (0.0%)	0.98	1/1954 (0.1%)

There are no bond-length outliers.

All angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	312	PHE	CA-CB-CG	-5.95	107.85	113.80

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	520	473	470	20
2	B	884	872	870	43
All	All	1404	1345	1340	58

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 21.

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:208:TRP:HE1	2:B:328:GLY:C	0.79	1.85
2:B:306:VAL:O	2:B:306:VAL:HG23	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:305:TYR:C	2:B:305:TYR:CD1	0.52	2.86
2:B:332:ARG:O	2:B:333:LEU:C	0.52	2.53
2:B:306:VAL:O	2:B:306:VAL:CG2	0.52	2.55
2:B:331:THR:O	2:B:332:ARG:O	0.52	2.27
2:B:273:TYR:CD1	2:B:273:TYR:N	0.50	2.79
2:B:324:TYR:O	2:B:325:ASN:C	0.50	2.54
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
1:A:184:THR:CG2	1:A:185:ASN:N	0.49	2.75
1:A:208:TRP:NE1	2:B:328:GLY:C	0.49	2.66
2:B:239:TRP:CD1	2:B:239:TRP:H	0.49	2.25
2:B:262:PHE:C	2:B:262:PHE:CD1	0.49	2.91
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:299:ASP:C	2:B:301:PRO:O	0.49	2.56
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
1:A:185:ASN:HD22	2:B:332:ARG:NH1	0.47	2.07
2:B:333:LEU:H	2:B:333:LEU:CD1	0.47	2.22
1:A:198:TYR:CD1	1:A:198:TYR:N	0.47	2.82
2:B:286:ASN:O	2:B:286:ASN:OD1	0.47	2.33
1:A:208:TRP:CD1	1:A:208:TRP:N	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
2:B:278:PHE:CD1	2:B:278:PHE:C	0.46	2.89
1:A:208:TRP:NE1	2:B:328:GLY:CA	0.45	2.79
1:A:189:GLU:CD	1:A:208:TRP:CH2	0.45	2.94
2:B:321:TYR:CD1	2:B:321:TYR:C	0.45	2.95
2:B:281:ALA:O	2:B:282:ILE:O	0.45	2.35
2:B:297:THR:O	2:B:297:THR:OG1	0.45	2.34
2:B:306:VAL:O	2:B:307:ALA:HB2	0.44	2.12
1:A:184:THR:OG1	1:A:190:LEU:C	0.44	2.60

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:255:ASP:OD1	2:B:255:ASP:O	0.43	2.36
2:B:295:LYS:O	2:B:303:ARG:O	0.43	2.37
2:B:313:ASP:O	2:B:313:ASP:CG	0.42	2.62
2:B:325:ASN:ND2	2:B:325:ASN:N	0.42	2.67
2:B:271:GLY:O	2:B:272:THR:OG1	0.42	2.35
2:B:307:ALA:C	2:B:309:LYS:N	0.42	2.78
2:B:312:PHE:CZ	2:B:321:TYR:CD2	0.42	3.08
2:B:333:LEU:H	2:B:333:LEU:HD12	0.42	1.74
2:B:307:ALA:C	2:B:309:LYS:H	0.41	2.23
2:B:318:LEU:HD23	2:B:322:HIS:HD1	0.41	1.75
2:B:271:GLY:C	2:B:272:THR:OG1	0.41	2.64
1:A:217:HIS:CD2	1:A:217:HIS:N	0.41	2.89
2:B:333:LEU:CD1	2:B:333:LEU:N	0.41	2.83
2:B:237:TYR:CG	2:B:239:TRP:CZ2	0.40	3.08
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	61/63 (97%)	53 (87%)	8 (13%)	0 (0%)	100	100
2	B	106/110 (96%)	81 (76%)	15 (14%)	10 (9%)	1	10
All	All	167/173 (97%)	134 (80%)	23 (14%)	10 (6%)	2	19

All 10 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	B	233	ASN
2	B	273	TYR
2	B	282	ILE
2	B	298	ASN
2	B	301	PRO
2	B	302	LYS
2	B	303	ARG

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Mol	Chain	Res	Type
2	B	307	ALA
2	B	325	ASN
2	B	332	ARG

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	57/57 (100%)	51 (89%)	6 (11%)	9	52
2	B	97/98 (99%)	87 (90%)	10 (10%)	9	53
All	All	154/155 (99%)	138 (90%)	16 (10%)	9	53

All 16 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	170	SER
1	A	173	GLU
1	A	200	LEU
1	A	214	LYS
1	A	224	SER
1	A	227	VAL
2	B	238	GLU
2	B	267	SER
2	B	269	THR
2	B	294	ILE
2	B	297	THR
2	B	313	ASP
2	B	321	TYR
2	B	325	ASN
2	B	329	LEU
2	B	330	VAL

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 oligosaccharides 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

No chemical shift data were provided