



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 01:54 PM BST

PDB ID : 1BLJ
Title : NMR ENSEMBLE OF BLK SH2 DOMAIN, 20 STRUCTURES
Authors : Metzler, W.J.; Leiting, B.; Pryor, K.; Mueller, L.; Farmer II, B.T.
Deposited on : 1996-03-26

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

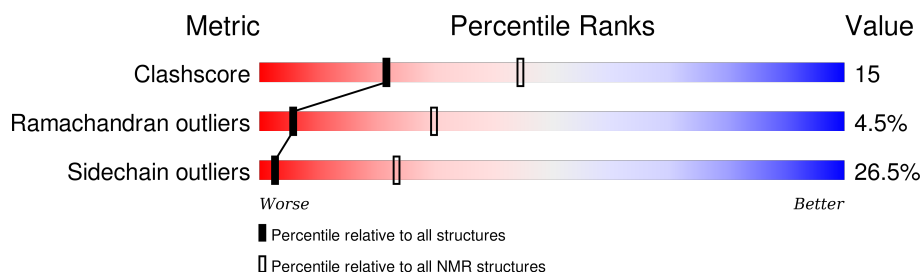
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	114	

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models).

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:13-A:111 (99)	0.44	10

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1816 atoms, of which 919 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called P55 BLK PROTEIN TYROSINE KINASE.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1816	571	919	156	167	3	

There are 3 discrepancies between the modelled and reference sequences:

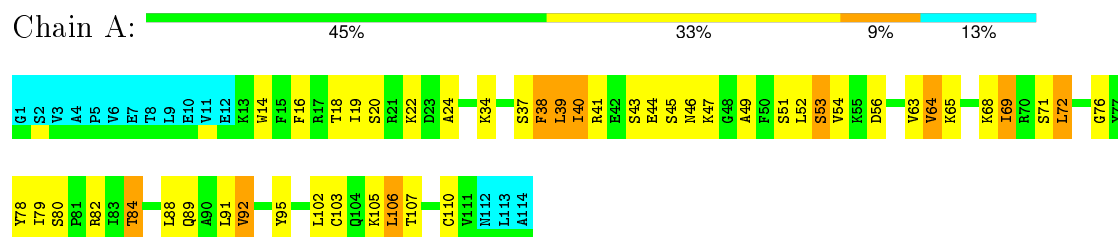
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	PRO	CONFLICT	UNP P16277
A	?	-	ASN	DELETION	UNP P16277
A	?	-	PHE	DELETION	UNP P16277

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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: P55 BLK PROTEIN TYROSINE KINASE

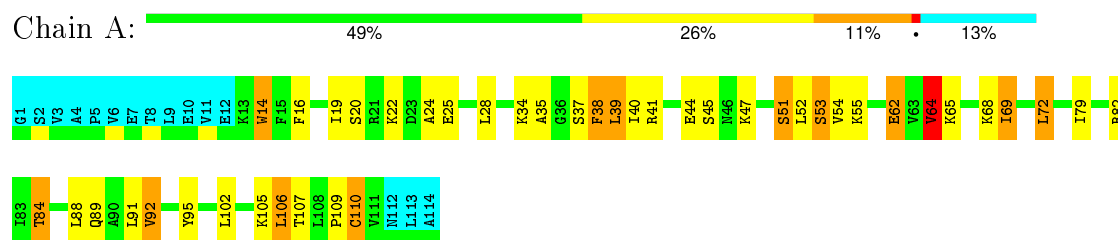


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

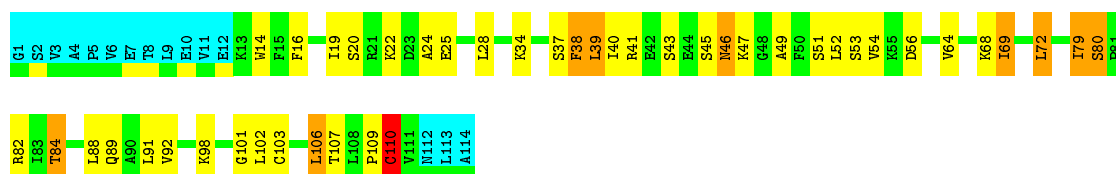
- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



4.2.2 Score per residue for model 2

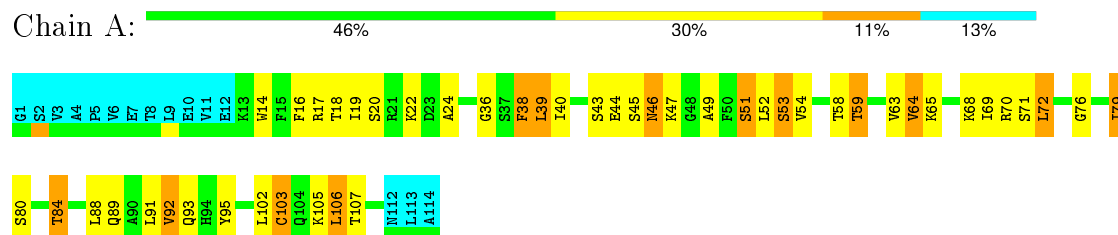
- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE





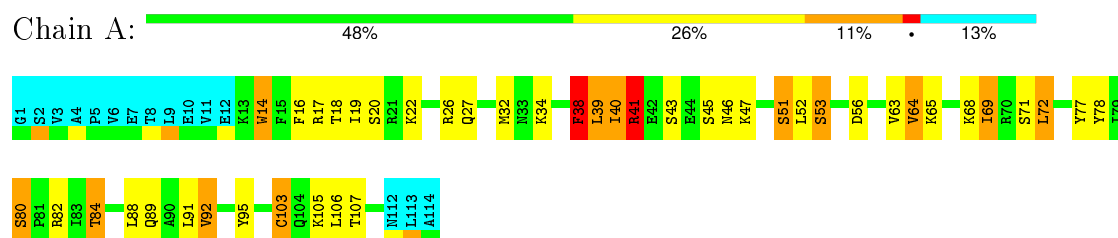
4.2.3 Score per residue for model 3

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



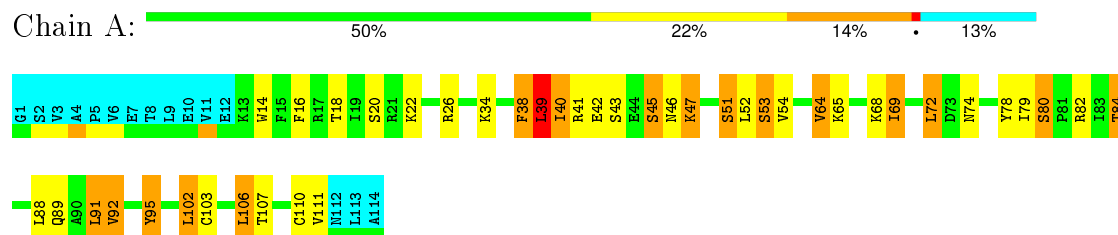
4.2.4 Score per residue for model 4

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



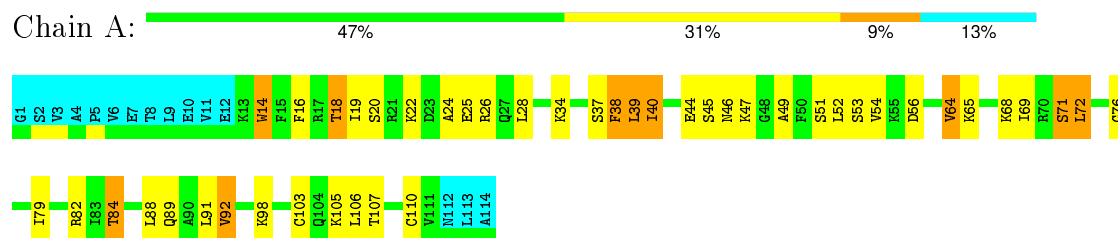
4.2.5 Score per residue for model 5

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



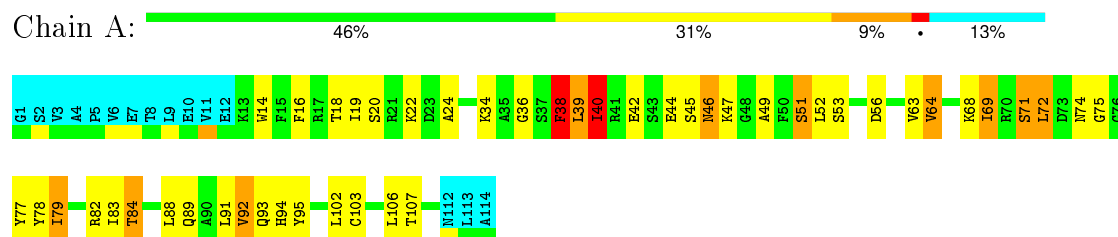
4.2.6 Score per residue for model 6

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



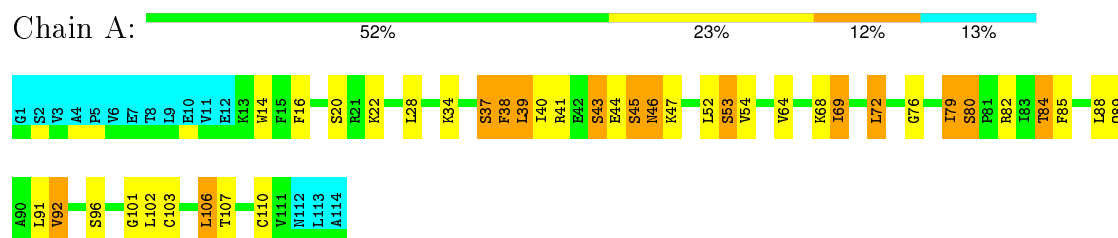
4.2.7 Score per residue for model 7

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



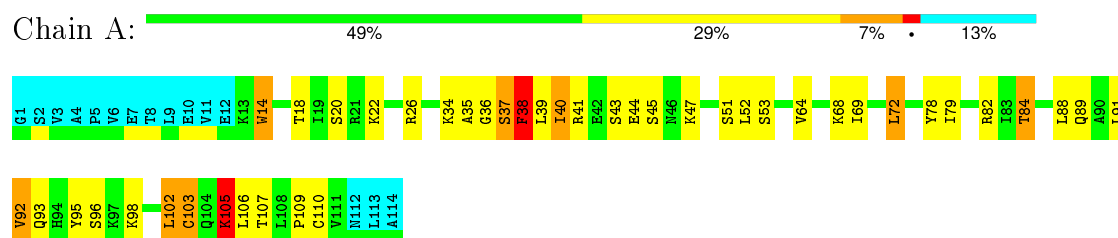
4.2.8 Score per residue for model 8

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



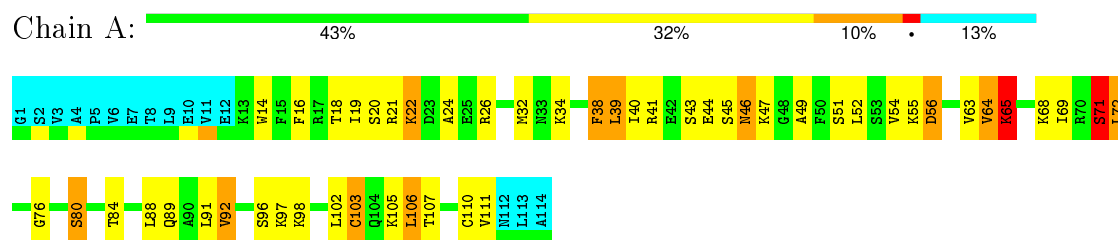
4.2.9 Score per residue for model 9

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



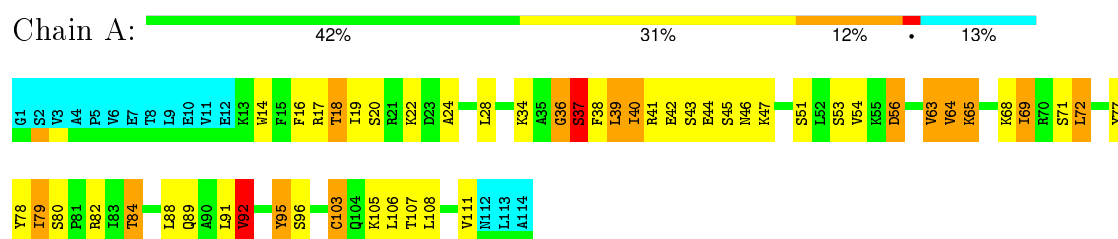
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



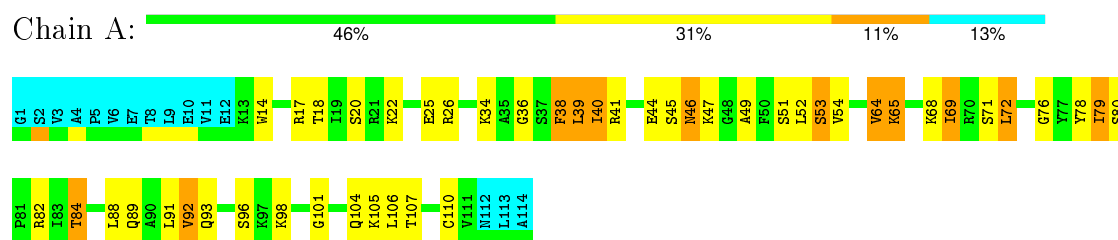
4.2.11 Score per residue for model 11

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



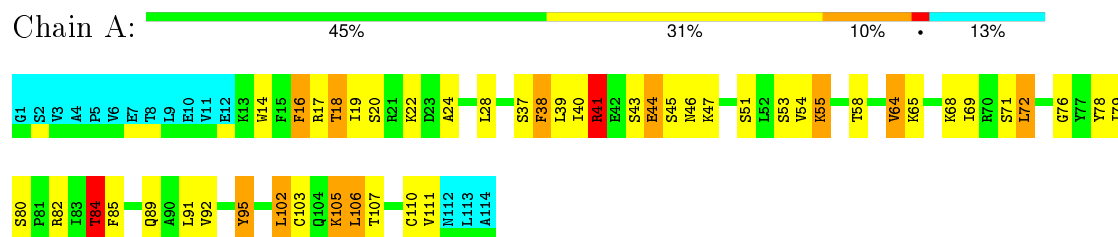
4.2.12 Score per residue for model 12

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



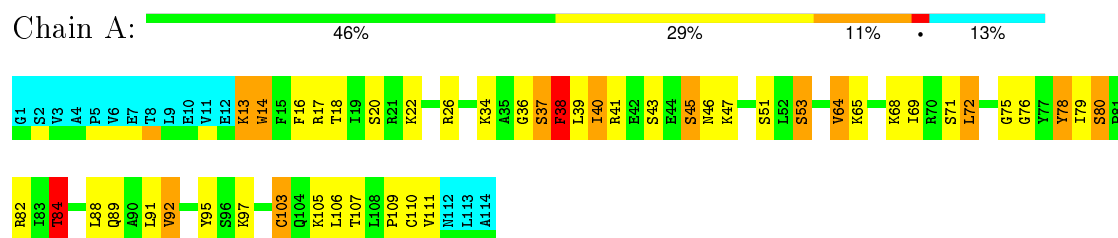
4.2.13 Score per residue for model 13

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



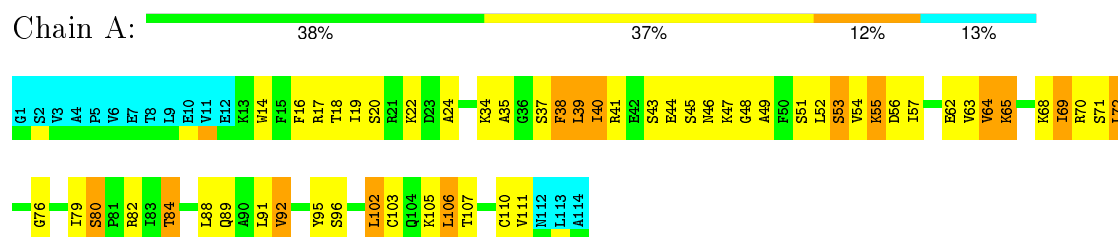
4.2.14 Score per residue for model 14

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



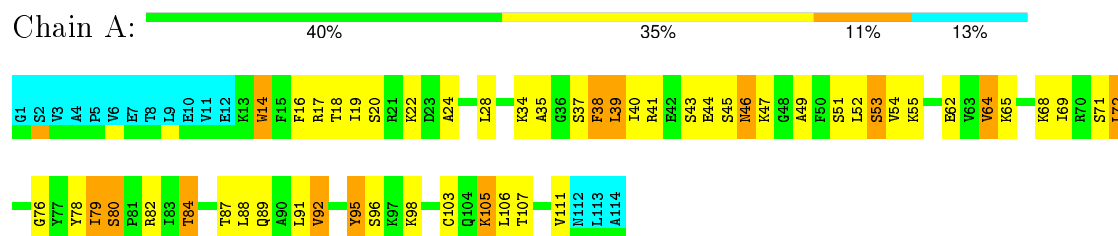
4.2.15 Score per residue for model 15

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



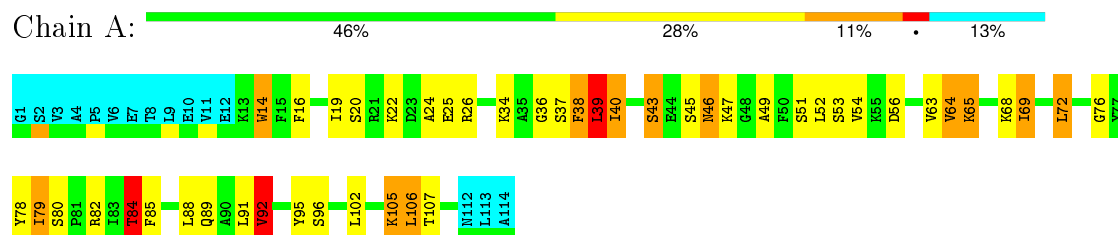
4.2.16 Score per residue for model 16

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



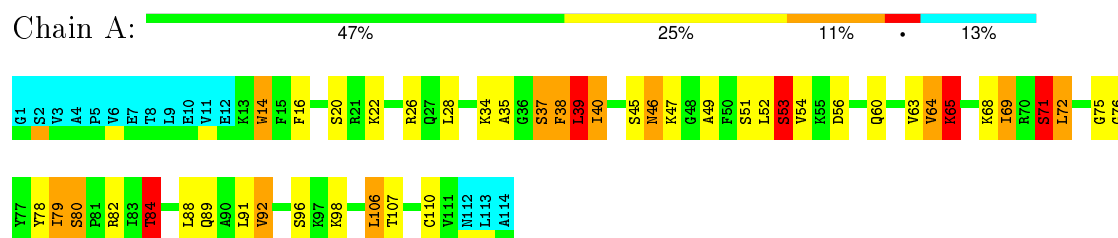
4.2.17 Score per residue for model 17

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



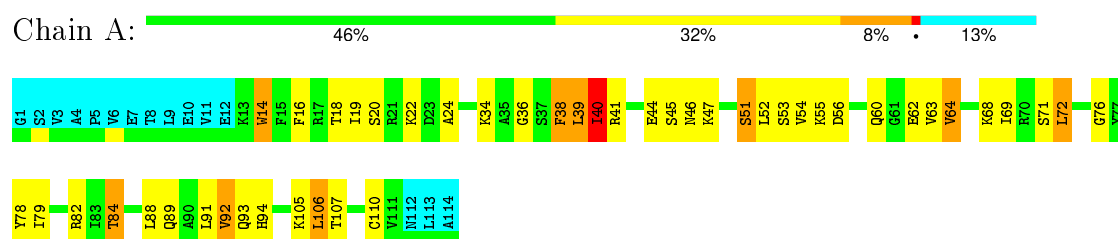
4.2.18 Score per residue for model 18

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



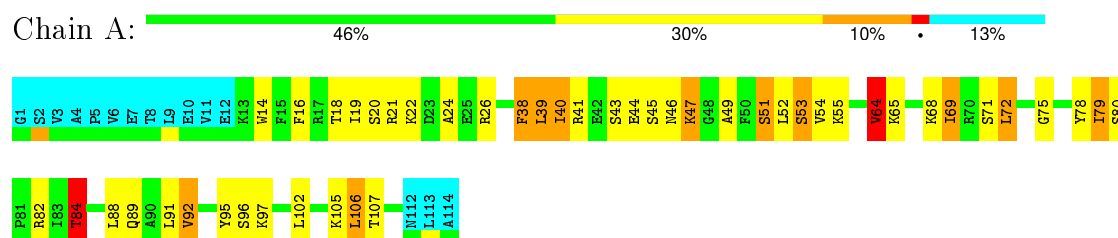
4.2.19 Score per residue for model 19

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



4.2.20 Score per residue for model 20

- Molecule 1: P55 BLK PROTEIN TYROSINE KINASE



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

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

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	0.95±0.01	7±1/807 (0.8±0.2%)	1.48±0.04	8±2/1086 (0.8±0.2%)
All	All	0.95	135/16140 (0.8%)	1.48	163/21720 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.3±0.5
All	All	0	7

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	20	SER	CB-OG	5.99	1.50	1.42	14	20
1	A	45	SER	CB-OG	5.86	1.49	1.42	16	20
1	A	37	SER	CB-OG	5.84	1.49	1.42	11	9
1	A	53	SER	CB-OG	5.54	1.49	1.42	11	19
1	A	43	SER	CB-OG	5.53	1.49	1.42	9	14
1	A	51	SER	CB-OG	5.48	1.49	1.42	16	14
1	A	71	SER	CB-OG	5.47	1.49	1.42	6	14
1	A	80	SER	CB-OG	5.32	1.49	1.42	15	15
1	A	96	SER	CB-OG	5.30	1.49	1.42	17	10

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	41	ARG	NE-CZ-NH1	12.58	126.59	120.30	4	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	37	SER	N-CA-CB	-8.16	98.27	110.50	11	1
1	A	38	PHE	CB-CG-CD1	7.77	126.24	120.80	6	14
1	A	45	SER	N-CA-CB	-7.46	99.30	110.50	8	4
1	A	38	PHE	C-N-CA	7.41	140.22	121.70	12	5
1	A	38	PHE	CB-CA-C	-7.34	95.72	110.40	7	4
1	A	65	LYS	N-CA-CB	7.32	123.77	110.60	10	6
1	A	95	TYR	CB-CG-CD2	-7.16	116.71	121.00	14	4
1	A	92	VAL	CA-CB-CG2	7.16	121.63	110.90	9	2
1	A	107	THR	CA-CB-OG1	6.97	123.64	109.00	11	20
1	A	56	ASP	N-CA-CB	6.93	123.07	110.60	11	1
1	A	92	VAL	CG1-CB-CG2	-6.86	99.92	110.90	13	19
1	A	64	VAL	CB-CA-C	6.69	124.11	111.40	19	13
1	A	38	PHE	CB-CG-CD2	-6.35	116.35	120.80	6	5
1	A	64	VAL	CG1-CB-CG2	-6.23	100.94	110.90	1	11
1	A	95	TYR	CB-CG-CD1	5.94	124.57	121.00	14	3
1	A	14	TRP	N-CA-CB	5.79	121.03	110.60	9	2
1	A	84	THR	CA-CB-OG1	5.76	121.11	109.00	7	19
1	A	59	THR	N-CA-CB	5.74	121.20	110.30	3	1
1	A	40	ILE	CG1-CB-CG2	-5.61	99.05	111.40	4	6
1	A	13	LYS	CA-C-N	-5.61	104.85	117.20	14	1
1	A	16	PHE	CB-CG-CD2	-5.56	116.91	120.80	13	2
1	A	39	LEU	CB-CG-CD2	5.51	120.37	111.00	13	1
1	A	109	PRO	C-N-CA	5.47	135.37	121.70	2	1
1	A	38	PHE	CA-C-N	-5.42	105.27	117.20	4	3
1	A	39	LEU	CB-CA-C	-5.38	99.97	110.20	5	3
1	A	13	LYS	C-N-CA	5.32	135.01	121.70	14	1
1	A	64	VAL	C-N-CA	5.19	134.67	121.70	15	2
1	A	46	ASN	CA-C-N	-5.08	106.03	117.20	8	1
1	A	36	GLY	N-CA-C	-5.08	100.41	113.10	11	1
1	A	69	ILE	CA-C-N	-5.07	106.05	117.20	17	1
1	A	55	LYS	N-CA-CB	-5.06	101.50	110.60	13	1
1	A	105	LYS	CB-CA-C	5.04	120.48	110.40	13	1
1	A	24	ALA	N-CA-CB	-5.03	103.06	110.10	13	1
1	A	47	LYS	CB-CA-C	5.02	120.43	110.40	5	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	95	TYR	Sidechain	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	38	PHE	Sidechain	1
1	A	77	TYR	Sidechain	1

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	790	812	812	24±6
All	All	15800	16240	16240	490

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:LEU:O	1:A:92:VAL:HG23	0.85	1.71	18	18
1:A:40:ILE:HD11	1:A:88:LEU:HD12	0.81	1.52	5	8
1:A:38:PHE:CE1	1:A:106:LEU:HD21	0.79	2.12	12	1
1:A:69:ILE:HG23	1:A:79:ILE:HG23	0.74	1.59	3	10
1:A:24:ALA:HB1	1:A:39:LEU:HD13	0.74	1.57	3	7
1:A:46:ASN:CG	1:A:49:ALA:HB3	0.74	2.01	20	9
1:A:40:ILE:HD12	1:A:52:LEU:HD13	0.73	1.60	19	8
1:A:24:ALA:HB1	1:A:39:LEU:CD1	0.71	2.16	15	7
1:A:38:PHE:CZ	1:A:106:LEU:HD21	0.71	2.21	12	1
1:A:19:ILE:CG2	1:A:24:ALA:HB2	0.69	2.17	2	12
1:A:39:LEU:O	1:A:52:LEU:HD12	0.69	1.87	19	13
1:A:38:PHE:CZ	1:A:106:LEU:CD2	0.69	2.75	5	15
1:A:40:ILE:CD1	1:A:88:LEU:HD12	0.66	2.21	20	8
1:A:72:LEU:H	1:A:72:LEU:HD22	0.64	1.51	8	4
1:A:38:PHE:CD2	1:A:52:LEU:HD11	0.63	2.28	12	11
1:A:38:PHE:CE1	1:A:54:VAL:HG13	0.63	2.28	2	14
1:A:28:LEU:HD21	1:A:110:CYS:SG	0.63	2.32	2	2
1:A:38:PHE:CE2	1:A:92:VAL:HG11	0.63	2.29	9	1
1:A:56:ASP:O	1:A:63:VAL:HG22	0.62	1.94	7	5
1:A:38:PHE:CD1	1:A:54:VAL:HG22	0.62	2.29	12	4
1:A:46:ASN:OD1	1:A:49:ALA:HB3	0.62	1.94	20	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:PHE:CE1	1:A:106:LEU:HD22	0.61	2.30	14	14
1:A:64:VAL:HG12	1:A:65:LYS:H	0.60	1.57	13	7
1:A:38:PHE:HD2	1:A:52:LEU:HD11	0.60	1.55	5	12
1:A:46:ASN:ND2	1:A:49:ALA:HB3	0.59	2.12	15	7
1:A:72:LEU:HD22	1:A:72:LEU:H	0.59	1.56	11	13
1:A:36:GLY:O	1:A:54:VAL:HG13	0.59	1.98	11	1
1:A:40:ILE:CD1	1:A:52:LEU:HD13	0.58	2.27	2	5
1:A:41:ARG:NH1	1:A:41:ARG:HB3	0.58	2.13	4	2
1:A:38:PHE:CD1	1:A:106:LEU:HD22	0.58	2.34	14	3
1:A:72:LEU:N	1:A:72:LEU:HD22	0.57	2.14	17	8
1:A:38:PHE:CE1	1:A:54:VAL:CG1	0.57	2.87	2	14
1:A:19:ILE:HG22	1:A:41:ARG:HH11	0.57	1.59	13	1
1:A:38:PHE:CD2	1:A:54:VAL:HG22	0.57	2.35	11	1
1:A:19:ILE:HG22	1:A:41:ARG:NH1	0.57	2.15	4	2
1:A:41:ARG:HH11	1:A:41:ARG:HB3	0.56	1.61	4	1
1:A:14:TRP:CH2	1:A:92:VAL:HG21	0.56	2.35	4	6
1:A:78:TYR:HB3	1:A:84:THR:HG23	0.55	1.76	20	3
1:A:106:LEU:N	1:A:106:LEU:HD23	0.55	2.16	19	6
1:A:72:LEU:HD22	1:A:72:LEU:N	0.54	2.17	11	8
1:A:40:ILE:N	1:A:41:ARG:HH21	0.54	2.01	13	1
1:A:14:TRP:HB3	1:A:109:PRO:CB	0.54	2.33	9	1
1:A:38:PHE:CE2	1:A:106:LEU:CD2	0.53	2.91	11	10
1:A:102:LEU:O	1:A:103:CYS:SG	0.53	2.67	13	6
1:A:69:ILE:HD12	1:A:88:LEU:HD11	0.52	1.82	4	2
1:A:24:ALA:O	1:A:39:LEU:HD11	0.52	2.05	20	2
1:A:106:LEU:HD23	1:A:106:LEU:N	0.52	2.20	6	2
1:A:38:PHE:CE1	1:A:106:LEU:CD2	0.52	2.93	13	4
1:A:36:GLY:O	1:A:38:PHE:CE1	0.51	2.64	14	2
1:A:69:ILE:CG2	1:A:79:ILE:HG23	0.51	2.35	3	1
1:A:36:GLY:O	1:A:106:LEU:HD23	0.51	2.06	12	1
1:A:75:GLY:O	1:A:84:THR:HG22	0.50	2.06	18	3
1:A:43:SER:HB3	1:A:46:ASN:OD1	0.50	2.05	17	1
1:A:38:PHE:CZ	1:A:106:LEU:HD22	0.50	2.41	19	6
1:A:79:ILE:HD12	1:A:102:LEU:HD21	0.50	1.84	1	2
1:A:38:PHE:CD1	1:A:106:LEU:HD21	0.50	2.41	12	1
1:A:38:PHE:CE2	1:A:106:LEU:HD22	0.50	2.42	19	2
1:A:40:ILE:O	1:A:40:ILE:HG23	0.49	2.07	16	3
1:A:54:VAL:O	1:A:64:VAL:HA	0.49	2.07	18	7
1:A:95:TYR:HB2	1:A:106:LEU:HD12	0.49	1.83	4	1
1:A:37:SER:HA	1:A:108:LEU:O	0.48	2.08	11	1
1:A:38:PHE:CE2	1:A:106:LEU:HD21	0.48	2.43	17	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HB3	1:A:41:ARG:HH21	0.48	1.68	4	1
1:A:72:LEU:HD11	1:A:78:TYR:CD2	0.48	2.43	9	5
1:A:40:ILE:HD11	1:A:88:LEU:CD1	0.48	2.35	7	8
1:A:28:LEU:HD22	1:A:37:SER:O	0.48	2.07	11	6
1:A:92:VAL:HG13	1:A:106:LEU:CD1	0.48	2.39	9	1
1:A:72:LEU:HD11	1:A:78:TYR:CE2	0.47	2.45	16	2
1:A:69:ILE:HG23	1:A:79:ILE:CG2	0.47	2.37	3	1
1:A:19:ILE:HG21	1:A:24:ALA:HB2	0.47	1.86	15	2
1:A:40:ILE:CG2	1:A:40:ILE:O	0.47	2.62	16	12
1:A:28:LEU:HD11	1:A:39:LEU:HG	0.47	1.86	11	1
1:A:24:ALA:CB	1:A:39:LEU:HD13	0.47	2.34	3	2
1:A:36:GLY:O	1:A:37:SER:C	0.47	2.53	11	1
1:A:39:LEU:HD12	1:A:53:SER:HB2	0.47	1.86	15	3
1:A:69:ILE:HG22	1:A:77:TYR:HB3	0.46	1.87	4	2
1:A:65:LYS:CE	1:A:103:CYS:SG	0.46	3.03	10	1
1:A:38:PHE:CZ	1:A:54:VAL:CG2	0.46	2.98	5	12
1:A:79:ILE:HD11	1:A:95:TYR:CZ	0.46	2.45	13	1
1:A:79:ILE:HD11	1:A:95:TYR:OH	0.46	2.10	16	2
1:A:71:SER:C	1:A:72:LEU:HD13	0.46	2.31	18	3
1:A:38:PHE:CE1	1:A:54:VAL:HG22	0.46	2.45	12	2
1:A:91:LEU:HD23	1:A:92:VAL:CG2	0.46	2.41	5	1
1:A:40:ILE:HG23	1:A:40:ILE:O	0.46	2.11	3	1
1:A:63:VAL:HG22	1:A:64:VAL:H	0.45	1.71	11	1
1:A:79:ILE:HD11	1:A:95:TYR:CE2	0.45	2.45	5	5
1:A:40:ILE:CG1	1:A:52:LEU:HD13	0.45	2.41	5	1
1:A:28:LEU:CD2	1:A:110:CYS:SG	0.45	3.02	2	2
1:A:36:GLY:HA2	1:A:105:LYS:O	0.45	2.11	9	4
1:A:40:ILE:CD1	1:A:88:LEU:CD1	0.45	2.95	20	7
1:A:14:TRP:CZ3	1:A:92:VAL:HG21	0.45	2.47	1	3
1:A:84:THR:C	1:A:85:PHE:CD1	0.44	2.90	13	2
1:A:53:SER:HA	1:A:65:LYS:O	0.44	2.12	18	1
1:A:39:LEU:CD2	1:A:110:CYS:SG	0.44	3.05	1	1
1:A:38:PHE:CE1	1:A:54:VAL:CG2	0.44	3.01	6	4
1:A:56:ASP:HB3	1:A:63:VAL:HG13	0.44	1.89	17	1
1:A:38:PHE:CD1	1:A:38:PHE:N	0.44	2.85	4	2
1:A:64:VAL:CG1	1:A:65:LYS:H	0.44	2.26	18	3
1:A:40:ILE:O	1:A:40:ILE:CG2	0.44	2.64	18	5
1:A:18:THR:HG22	1:A:42:GLU:HG2	0.43	1.88	5	1
1:A:56:ASP:HB2	1:A:63:VAL:CG1	0.43	2.43	11	1
1:A:38:PHE:CZ	1:A:106:LEU:HD23	0.43	2.48	11	1
1:A:43:SER:CB	1:A:46:ASN:OD1	0.43	2.66	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:VAL:HG23	1:A:64:VAL:O	0.43	2.12	7	1
1:A:91:LEU:HD23	1:A:92:VAL:HG23	0.43	1.91	5	1
1:A:38:PHE:CZ	1:A:54:VAL:HG21	0.43	2.49	17	3
1:A:38:PHE:CE1	1:A:106:LEU:HB3	0.43	2.49	14	1
1:A:56:ASP:N	1:A:63:VAL:O	0.43	2.52	10	1
1:A:40:ILE:HG21	1:A:88:LEU:HD13	0.42	1.90	10	1
1:A:40:ILE:N	1:A:41:ARG:NH2	0.42	2.67	4	1
1:A:38:PHE:CE2	1:A:92:VAL:HG13	0.42	2.50	4	1
1:A:24:ALA:HB1	1:A:39:LEU:HG	0.42	1.91	17	1
1:A:38:PHE:O	1:A:110:CYS:SG	0.42	2.77	2	1
1:A:110:CYS:SG	1:A:111:VAL:N	0.42	2.93	5	1
1:A:76:GLY:CA	1:A:85:PHE:O	0.42	2.68	8	1
1:A:28:LEU:O	1:A:55:LYS:CE	0.42	2.68	16	1
1:A:79:ILE:HD11	1:A:95:TYR:HE2	0.42	1.74	1	1
1:A:72:LEU:CD2	1:A:72:LEU:N	0.41	2.83	11	1
1:A:92:VAL:HG13	1:A:106:LEU:HD13	0.41	1.91	9	1
1:A:72:LEU:N	1:A:72:LEU:HD13	0.41	2.29	1	1
1:A:93:GLN:CG	1:A:94:HIS:N	0.41	2.83	19	2
1:A:55:LYS:HG2	1:A:57:ILE:HD11	0.41	1.92	15	1
1:A:46:ASN:HB2	1:A:49:ALA:H	0.41	1.76	16	1
1:A:36:GLY:C	1:A:38:PHE:CE1	0.41	2.93	11	1
1:A:35:ALA:HB2	1:A:57:ILE:HG12	0.41	1.93	15	1
1:A:38:PHE:CZ	1:A:106:LEU:HA	0.41	2.51	11	1
1:A:43:SER:O	1:A:45:SER:N	0.41	2.53	8	1
1:A:24:ALA:HB3	1:A:25:GLU:OE1	0.41	2.16	2	1
1:A:36:GLY:O	1:A:106:LEU:CD2	0.41	2.69	12	1
1:A:22:LYS:CD	1:A:22:LYS:C	0.40	2.90	10	1

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	99/114 (87%)	80±3 (81±3%)	14±3 (14±3%)	5±2 (5±2%)	6	30
All	All	1980/2280 (87%)	1603 (81%)	287 (14%)	90 (5%)	6	30

All 25 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	110	CYS	12
1	A	76	GLY	11
1	A	103	CYS	9
1	A	17	ARG	7
1	A	40	ILE	7
1	A	111	VAL	5
1	A	44	GLU	4
1	A	35	ALA	4
1	A	105	LYS	4
1	A	64	VAL	3
1	A	18	THR	3
1	A	102	LEU	3
1	A	101	GLY	3
1	A	109	PRO	2
1	A	45	SER	2
1	A	63	VAL	2
1	A	59	THR	1
1	A	75	GLY	1
1	A	14	TRP	1
1	A	47	LYS	1
1	A	37	SER	1
1	A	62	GLU	1
1	A	13	LYS	1
1	A	48	GLY	1
1	A	104	GLN	1

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	87/99 (88%)	64±2 (74±2%)	23±2 (26±2%)	3	23
All	All	1740/1980 (88%)	1279 (74%)	461 (26%)	3	23

All 53 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	84	THR	20
1	A	89	GLN	20
1	A	22	LYS	20
1	A	68	LYS	20
1	A	47	LYS	20
1	A	91	LEU	20
1	A	72	LEU	20
1	A	69	ILE	19
1	A	39	LEU	19
1	A	14	TRP	18
1	A	82	ARG	18
1	A	16	PHE	17
1	A	34	LYS	17
1	A	46	ASN	15
1	A	41	ARG	15
1	A	79	ILE	14
1	A	18	THR	14
1	A	106	LEU	12
1	A	51	SER	12
1	A	44	GLU	11
1	A	105	LYS	11
1	A	26	ARG	10
1	A	80	SER	9
1	A	53	SER	8
1	A	98	LYS	7
1	A	55	LYS	6
1	A	65	LYS	6
1	A	78	TYR	5
1	A	102	LEU	5
1	A	62	GLU	4
1	A	38	PHE	4
1	A	103	CYS	4
1	A	25	GLU	4
1	A	71	SER	3
1	A	97	LYS	3
1	A	93	GLN	3
1	A	56	ASP	3
1	A	58	THR	2
1	A	21	ARG	2
1	A	60	GLN	2
1	A	74	ASN	2
1	A	92	VAL	2
1	A	37	SER	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	40	ILE	2
1	A	70	ARG	2
1	A	42	GLU	2
1	A	111	VAL	1
1	A	87	THR	1
1	A	27	GLN	1
1	A	17	ARG	1
1	A	83	ILE	1
1	A	110	CYS	1
1	A	32	MET	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 carbohydrates 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