



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2LSP / pdb_00002lsp
BMRB ID : 18439
Title : solution structures of BRD4 second bromodomain with NF-kB-K310ac peptide
Authors : Zhang, G.; Liu, R.; Zhong, Y.; Plotnikov, A.N.; Zhang, W.; Rusinova, E.;
Gerona-Nevarro, G.; Moshkina, N.; Joshua, J.; Chuang, P.Y.; Ohlmeyer, M.;
He, J.; Zhou, M.-M.
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<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
Mogul : 2022.3.0, CSD as543be (2022)
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

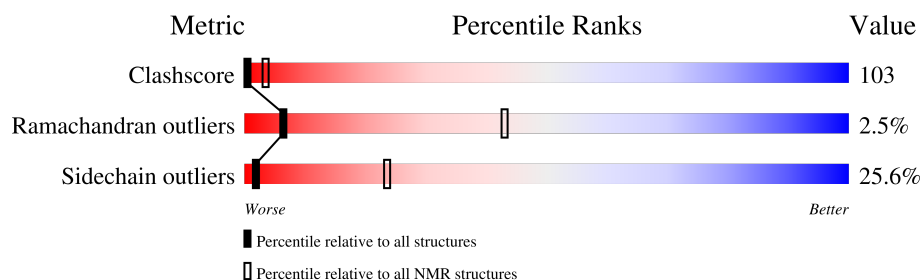
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

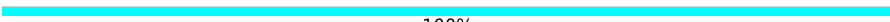
The overall completeness of chemical shifts assignment is 79%.

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	13	 100%
2	B	128	 14%48%18%20%

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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	B:353-B:454 (102)	0.17	17

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 and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2294 atoms, of which 1141 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NF-kB-K310ac peptide.

Mol	Chain	Residues	Atoms						Trace
1	A	13	Total	C	H	N	O	S	0
			239	74	123	19	22	1	

- Molecule 2 is a protein called Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms						Trace
2	B	128	Total	C	H	N	O	S	0
			2055	658	1018	175	193	11	

4 Residue-property plots

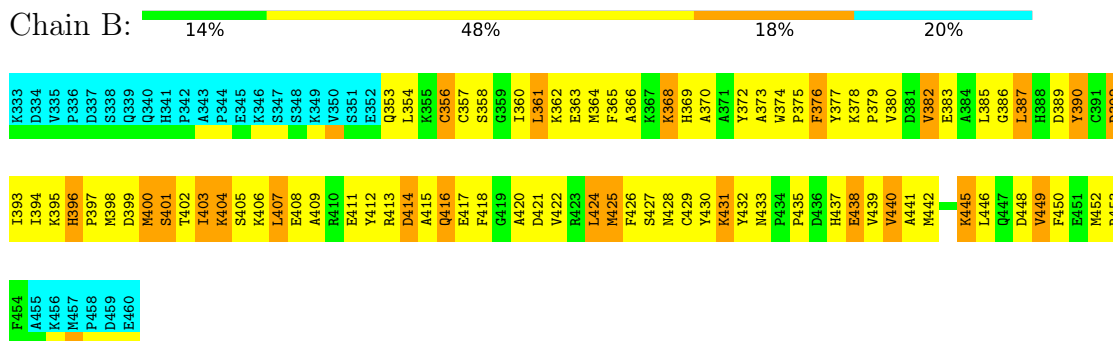
4.1 Average score per residue in the NMR ensemble

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: NF-kB-K310ac peptide



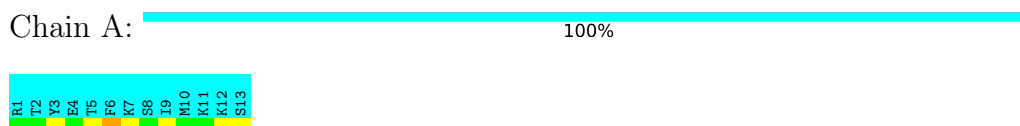
- Molecule 2: Bromodomain-containing protein 4



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

The representative model is number 17. Colouring as in section 4.1 above.

- Molecule 1: NF-kB-K310ac peptide



- Molecule 2: Bromodomain-containing protein 4



I393	K333
I394	D334
K395	V335
H396	P336
M397	D337
M398	S338
D399	Q339
M400	Q340
S401	H341
T402	P342
I403	A343
K404	P344
S405	E345
K406	K346
L407	S347
E408	K349
A409	V350
R410	S351
E411	E352
Y412	Q353
R413	L354
D414	K355
A415	C356
Q416	C357
E417	S358
F418	G359
G419	I360
A420	L361
D421	K362
V422	E363
R423	K364
L424	F365
M425	A366
F426	K367
S427	S368
N428	H369
C429	I370
Y430	A371
K431	Y372
Y432	A373
N433	W374
P434	P375
P435	F376
D436	Y377
H437	K378
E438	P379
V439	V380
V440	D381
A441	V382
M442	E383
A443	A384
R444	L385
K445	G386
L446	L387
Q447	K388
D448	D389
V449	Y390
F450	C391
	D392
R453	

E454
A455
K456
M457
P458
D459
E460

5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing, torsion angle dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	refinement	2.3
TALOS	geometry optimization	3.70F1
CNS	structure solution	1.21
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section [7](#) of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1435
Number of shifts mapped to atoms	1435
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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: ALY

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
2	B	1.21±0.01	1±0/860 (0.1± 0.1%)	1.23±0.01	1±1/1157 (0.1± 0.1%)
All	All	1.21	11/17200 (0.1%)	1.23	22/23140 (0.1%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	407	LEU	N-CA	-5.23	1.40	1.46	17	11

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
2	B	411	GLU	N-CA-C	-5.73	105.17	111.82	2	10
2	B	394	ILE	N-CA-CB	-5.40	106.83	112.06	9	9
2	B	413	ARG	N-CA-C	-5.19	105.74	111.71	4	1
2	B	424	LEU	N-CA-C	-5.12	105.40	111.69	19	2

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	0	0	0	0±0
2	B	837	825	821	171±7
All	All	16740	16500	16420	3412

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 103.

5 of 355 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:373:ALA:HB2	2:B:446:LEU:HD21	1.11	1.22	16	20
2:B:372:TYR:HA	2:B:442:MET:SD	0.92	2.03	17	20
2:B:372:TYR:CG	2:B:445:LYS:HD2	0.92	1.98	8	7
2:B:372:TYR:CD2	2:B:445:LYS:HG2	0.91	2.00	12	4
2:B:357:CYS:HB3	2:B:418:PHE:CD1	0.91	2.01	5	20

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	0	-	-	-	-	
2	B	102/128 (80%)	85±1 (83±1%)	15±1 (15±1%)	3±1 (3±1%)	6	43
All	All	2040/2820 (72%)	1691 (83%)	297 (15%)	52 (3%)	6	43

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

Mol	Chain	Res	Type	Models (Total)
2	B	387	LEU	20
2	B	390	TYR	12
2	B	414	ASP	12
2	B	373	ALA	7
2	B	367	LYS	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	0	-	-	-	
2	B	89/113 (79%)	66±2 (74±2%)	23±2 (26±2%)	2	23
All	All	1780/2500 (71%)	1324 (74%)	456 (26%)	2	23

5 of 42 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)
2	B	361	LEU	20
2	B	368	LYS	20
2	B	376	PHE	20
2	B	383	GLU	20
2	B	385	LEU	20

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	ALY	A	7	1	10,11,12	0.61±0.04	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles

that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	ALY	A	7	1	7,12,14	0.94±0.03	0±0 (0±3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ALY	A	7	1	-	0±0,9,10,12	-

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	7	ALY	CH3-CH-NZ	2.03	119.59	116.12	9	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1435
Number of shifts mapped to atoms	1435
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	19

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	127	-0.45 ± 0.26	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	123	0.33 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	10	—	None (insufficient data)
^{15}N	114	0.41 ± 0.37	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 1131 atoms were assigned a chemical shift out of a possible 1435. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	400/503 (80%)	195/202 (97%)	110/204 (54%)	95/97 (98%)
Sidechain	644/774 (83%)	428/502 (85%)	214/242 (88%)	2/30 (7%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	87/158 (55%)	44/76 (58%)	42/73 (58%)	1/9 (11%)
Overall	1131/1435 (79%)	667/780 (86%)	366/519 (71%)	98/136 (72%)

7.1.4 Statistically unusual chemical shifts [i](#)

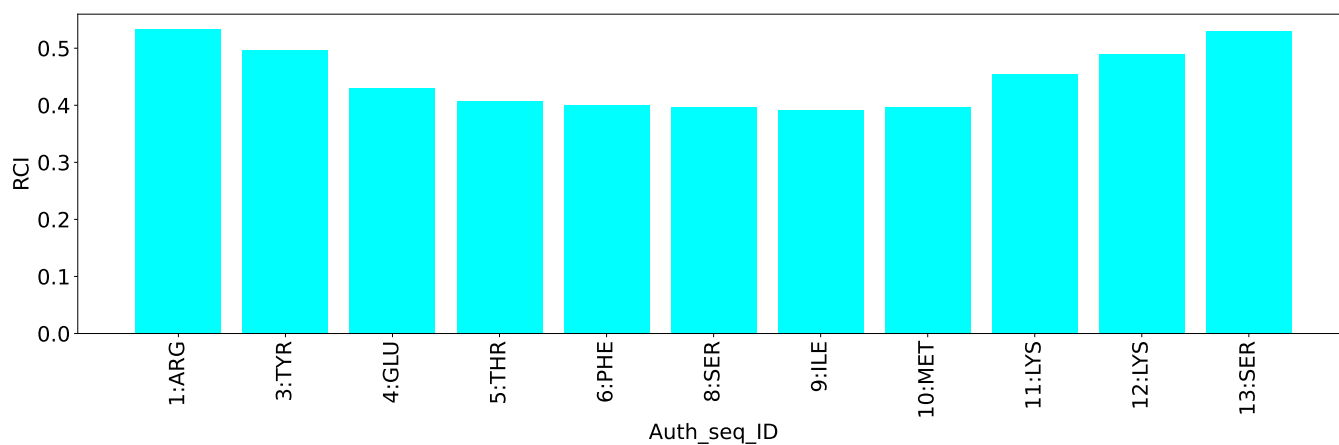
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	347	SER	C	8.45	166.15 – 183.14	-97.8
1	B	386	GLY	C	7.90	164.92 – 182.89	-92.4
1	B	385	LEU	C	7.48	167.56 – 186.66	-88.8
1	B	346	LYS	C	8.51	167.28 – 186.22	-88.8
1	B	447	GLN	C	11.57	166.94 – 185.80	-87.4
1	B	430	TYR	C	7.61	165.86 – 185.23	-86.7
1	B	388	HIS	C	8.30	165.57 – 184.97	-86.1
1	B	437	HIS	C	9.41	165.57 – 184.97	-85.5
1	B	384	ALA	C	7.86	167.61 – 188.05	-83.2
1	B	366	ALA	C	9.11	167.61 – 188.05	-82.5
1	B	375	PRO	HG2	-0.72	0.41 – 3.45	-8.7
1	B	447	GLN	HB2	0.07	0.80 – 3.29	-8.0
1	B	375	PRO	HB2	-0.35	0.37 – 3.78	-7.1
1	B	357	CYS	HB2	0.35	0.81 – 5.11	-6.1
1	B	375	PRO	HD2	1.62	1.93 – 5.38	-5.9
1	B	422	VAL	HG11	-0.67	-0.48 – 2.12	-5.7
1	B	422	VAL	HG12	-0.67	-0.48 – 2.12	-5.7
1	B	422	VAL	HG13	-0.67	-0.48 – 2.12	-5.7
1	B	439	VAL	H	11.70	4.98 – 11.56	5.2

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

