



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:40 PM GMT

PDB ID : 1LE5  
Title : Crystal structure of a NF-kB heterodimer bound to an IFN $\gamma$ -kB  
Authors : Berkowitz, B.; Huang, D.B.; Chen-Park, F.E.; Sigler, P.B.; Ghosh, G.  
Deposited on : 2002-04-09  
Resolution : 2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

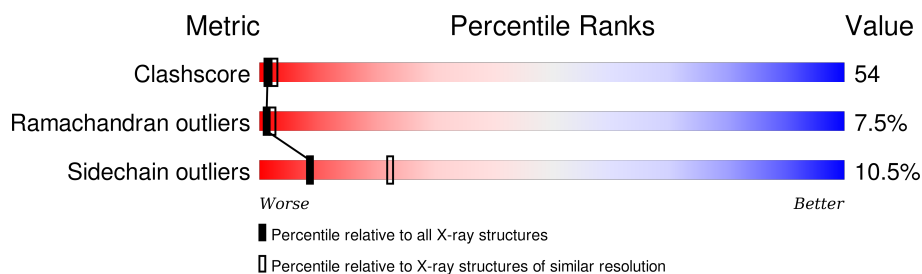
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	12	<div> <div>17%</div> <div>83%</div> </div>
1	G	12	<div> <div>50%</div> <div>33%</div> <div>17%</div> </div>
2	D	12	<div> <div>25%</div> <div>75%</div> </div>
2	H	12	<div> <div>25%</div> <div>8%</div> <div>67%</div> </div>
3	A	274	<div> <div>31%</div> <div>57%</div> <div>12%</div> <div>.</div> </div>
3	E	274	<div> <div>31%</div> <div>57%</div> <div>10%</div> <div>.</div> </div>
4	B	313	<div> <div>28%</div> <div>61%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	313	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (34%), yellow (52%), and orange (13%). A small red dot is at the end of the bar.

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10439 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called 5'-D(\*TP\*GP\*GP\*GP\*AP\*AP\*AP\*TP\*TP\*CP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			244	118	44	71	11			
1	G	12	Total	C	N	O	P	0	0	0
			244	118	44	71	11			

- Molecule 2 is a DNA chain called 5'-D(\*AP\*AP\*GP\*GP\*AP\*AP\*TP\*TP\*TP\*CP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			242	117	45	69	11			
2	H	12	Total	C	N	O	P	0	0	0
			242	117	45	69	11			

- Molecule 3 is a protein called Nuclear factor NF-kappa-B p65 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	274	Total	C	N	O	S	0	0	0
			2184	1361	402	409	12			
3	E	274	Total	C	N	O	S	0	0	0
			2184	1361	402	409	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	CLONING ARTIFACT	UNP Q04207
A	19	ALA	-	CLONING ARTIFACT	UNP Q04207
E	18	MET	-	CLONING ARTIFACT	UNP Q04207
E	19	ALA	-	CLONING ARTIFACT	UNP Q04207

- Molecule 4 is a protein called Nuclear factor NF-kappa-B p50 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	313	Total 2462	C 1559	N 429	O 461	S 13	0	0	0
4	F	313	Total 2462	C 1559	N 429	O 461	S 13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	38	MET	-	INITIATING MET	UNP P25799
F	38	MET	-	INITIATING MET	UNP P25799

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total 33	O 33	0	0
5	B	32	Total 32	O 32	0	0
5	C	4	Total 4	O 4	0	0
5	D	9	Total 9	O 9	0	0
5	E	32	Total 32	O 32	0	0
5	F	51	Total 51	O 51	0	0
5	G	6	Total 6	O 6	0	0
5	H	8	Total 8	O 8	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: 5'-D(\*TP\*GP\*GP\*GP\*AP\*AP\*AP\*TP\*TP\*CP\*CP\*T)-3'

Chain C: 



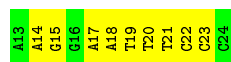
- Molecule 1: 5'-D(\*TP\*GP\*GP\*GP\*AP\*AP\*AP\*TP\*TP\*CP\*CP\*T)-3'

Chain G: 



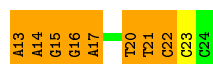
- Molecule 2: 5'-D(\*AP\*AP\*GP\*GP\*AP\*AP\*TP\*TP\*TP\*CP\*CP\*C)-3'

Chain D: 



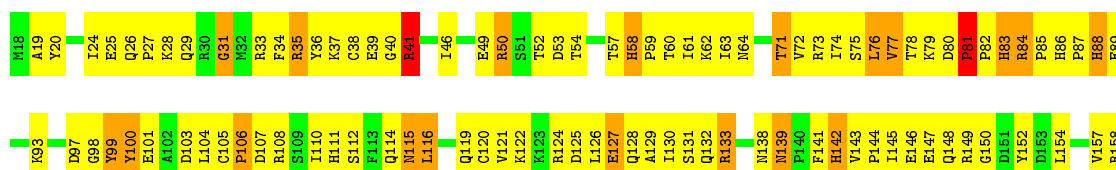
- Molecule 2: 5'-D(\*AP\*AP\*GP\*GP\*AP\*AP\*TP\*TP\*TP\*CP\*CP\*C)-3'

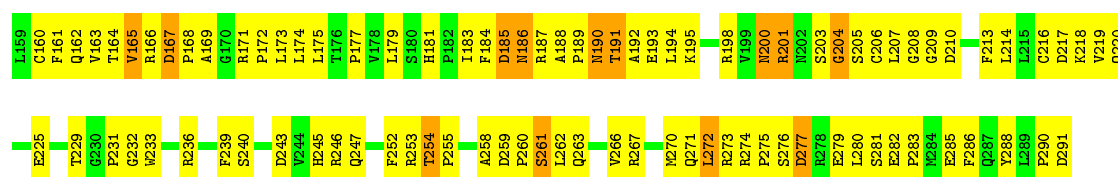
Chain H: 



- Molecule 3: Nuclear factor NF-kappa-B p65 subunit

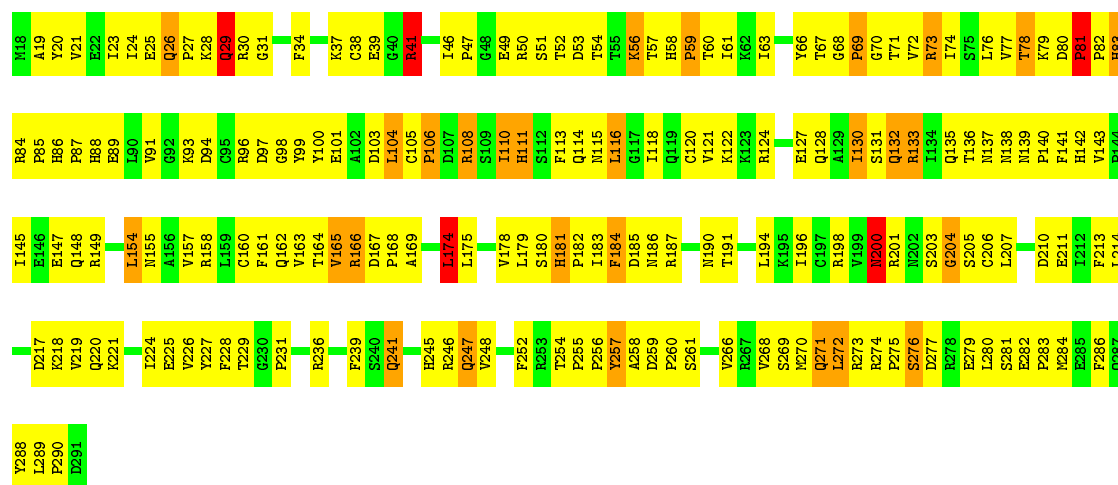
Chain A: 





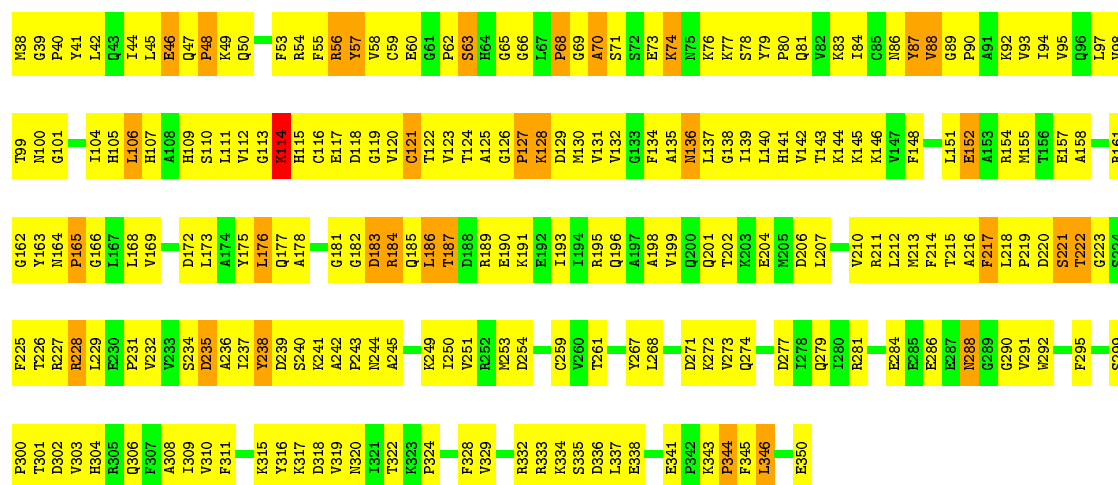
• Molecule 3: Nuclear factor NF-kappa-B p65 subunit

Chain E: 31% 57% 10%



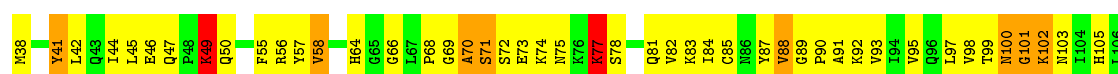
• Molecule 4: Nuclear factor NF-kappa-B p50 subunit

Chain B: 28% 61% 10%



• Molecule 4: Nuclear factor NF-kappa-B p50 subunit

Chain F: 34% 52% 13%



N320	D235	S171	H107
L321	A236	D172	A108
F322	I237	L173	H109
K323	Y238	A174	S110
V327	D239	Y175	L111
F328	S240	L176	V112
V329	N244	Q177	G113
	A245	A178	K114
	S246	E179	H115
R332	N247	G182	C116
K333	L248	D183	E117
S335	V249	R184	D118
D336	I250	Q185	G121
L337	D254	L186	T122
E338	R255	T187	V123
T339	C259	D188	T124
S340		R189	A125
E341		E190	G126
F342		K191	P127
K343	Y267	E192	M130
F345	L268	I193	V131
L346	D271	I194	V132
	V273	Q196	G133
P349	Q274	A197	F134
E350	K275	A198	A135
		V199	M136
		Q200	L137
		Q201	G138
		T202	T139
		K203	L140
		E204	H141
		M205	V142
		V209	T143
		V210	K144
			K145
			K146
			V147
			F148
			E149
			T150
			L151
			E152
			A153
			R154
			M155
			T156
			E157
			I160
			R161
			G162
			Y163
			N164
			P165
			G166
			L167
			H170



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.53Å 138.01Å 89.32Å 90.00° 97.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75	Depositor
% Data completeness (in resolution range)	88.0 (20.00-2.75)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.260 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

## 5 Model quality

### 5.1 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 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	C	0.32	0/273	0.74	0/420
1	G	0.69	0/273	1.26	3/420 (0.7%)
2	D	0.32	0/271	0.78	0/416
2	H	0.80	0/271	1.31	2/416 (0.5%)
3	A	0.39	0/2236	0.67	0/3031
3	E	0.39	0/2236	0.69	0/3031
4	B	0.35	0/2514	0.60	0/3394
4	F	0.41	0/2514	0.66	0/3394
All	All	0.41	0/10588	0.71	5/14522 (0.0%)

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 outliers	#Planarity outliers
1	G	0	5
2	H	0	6
All	All	0	11

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	8	DT	O4'-C4'-C3'	-5.71	102.22	104.50
2	H	17	DA	O4'-C1'-C2'	5.32	110.16	105.90
1	G	7	DA	O4'-C1'-C2'	5.27	110.11	105.90
1	G	5	DA	N9-C1'-C2'	5.21	122.49	112.60
2	H	15	DG	N9-C1'-C2'	5.10	122.29	112.60

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	11	DC	Sidechain
1	G	4	DG	Sidechain
1	G	5	DA	Sidechain
1	G	6	DA	Sidechain
1	G	7	DA	Sidechain

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	244	0	138	28	0
1	G	244	0	138	33	0
2	D	242	0	137	23	0
2	H	242	0	137	14	0
3	A	2184	0	2146	239	0
3	E	2184	0	2146	245	0
4	B	2462	0	2458	301	0
4	F	2462	0	2458	250	0
5	A	33	0	0	5	0
5	B	32	0	0	4	0
5	C	4	0	0	3	0
5	D	9	0	0	1	0
5	E	32	0	0	7	0
5	F	51	0	0	5	0
5	G	6	0	0	2	0
5	H	8	0	0	1	0
All	All	10439	0	9758	1074	0

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 54.

The worst 5 of 1074 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:DT:H3'	4:B:65:GLY:HA2	1.30	1.11
4:F:250:ILE:HG23	4:F:268:LEU:HD21	1.29	1.06
4:B:104:ILE:HG22	4:B:211:ARG:HH22	1.23	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:273:ARG:HD2	3:E:280:LEU:HD11	1.41	1.02
4:B:134:PHE:HB3	4:B:137:LEU:HD11	1.42	1.02

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	
3	A	272/274 (99%)	204 (75%)	49 (18%)	19 (7%)	1	3
3	E	272/274 (99%)	201 (74%)	50 (18%)	21 (8%)	1	2
4	B	311/313 (99%)	236 (76%)	54 (17%)	21 (7%)	1	3
4	F	311/313 (99%)	240 (77%)	44 (14%)	27 (9%)	1	1
All	All	1166/1174 (99%)	881 (76%)	197 (17%)	88 (8%)	1	2

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	81	PRO
3	A	83	HIS
3	A	115	ASN
3	A	204	GLY
4	B	101	GLY

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	
3	A	243/243 (100%)	218 (90%)	25 (10%)	9	23
3	E	243/243 (100%)	215 (88%)	28 (12%)	7	19
4	B	269/269 (100%)	244 (91%)	25 (9%)	11	29
4	F	269/269 (100%)	239 (89%)	30 (11%)	7	20
All	All	1024/1024 (100%)	916 (90%)	108 (10%)	8	22

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	341	GLU
3	E	108	ARG
4	F	227	ARG
3	E	20	TYR
3	E	56	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	279	GLN
3	E	111	HIS
4	F	170	HIS
4	B	288	ASN
4	B	330	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.