



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:09 PM UTC

PDB ID : 1LE9 / pdb_00001le9
Title : Crystal structure of a NF-kB heterodimer bound to the Ig/HIV-kB siti
Authors : Benjamin, B.; Huang, D.B.; Chen-Park, F.E.; Sigler, P.B.; Ghosh, G.
Deposited on : 2002-04-09
Resolution : 3.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

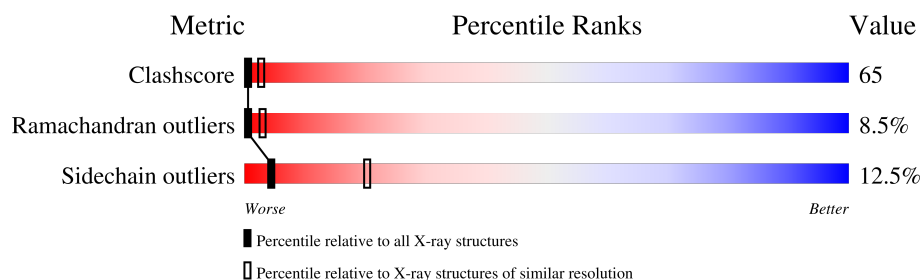
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	12	17% 83%
1	G	12	33% 67%
2	D	12	50% 50%
2	H	12	100%
3	A	274	21% 59% 18% .
3	E	274	26% 56% 16% .
4	B	313	28% 56% 14% .
4	F	313	30% 51% 17% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10232 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*CP*TP*TP*TP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			241	117	39	74	11			
1	G	12	Total	C	N	O	P	0	0	0
			241	117	39	74	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			245	117	51	66	11			
2	H	12	Total	C	N	O	P	0	0	0
			245	117	51	66	11			

- Molecule 3 is a protein called NUCLEAR FACTOR NF-KAPPA-B P65 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	273	Total	C	N	O	S	0	0	0
			2176	1356	401	408	11			
3	E	273	Total	C	N	O	S	0	0	0
			2176	1356	401	408	11			

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.

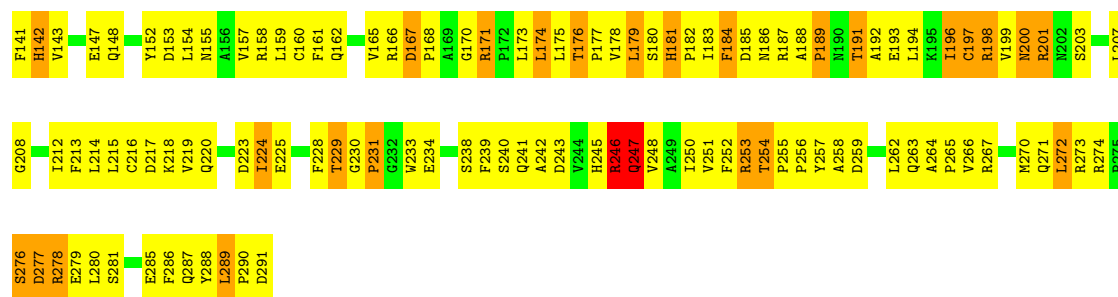
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	312	Total 2454	C 1554	N 428	O 460	S 12	0	0	0
4	F	312	Total 2454	C 1554	N 428	O 460	S 12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

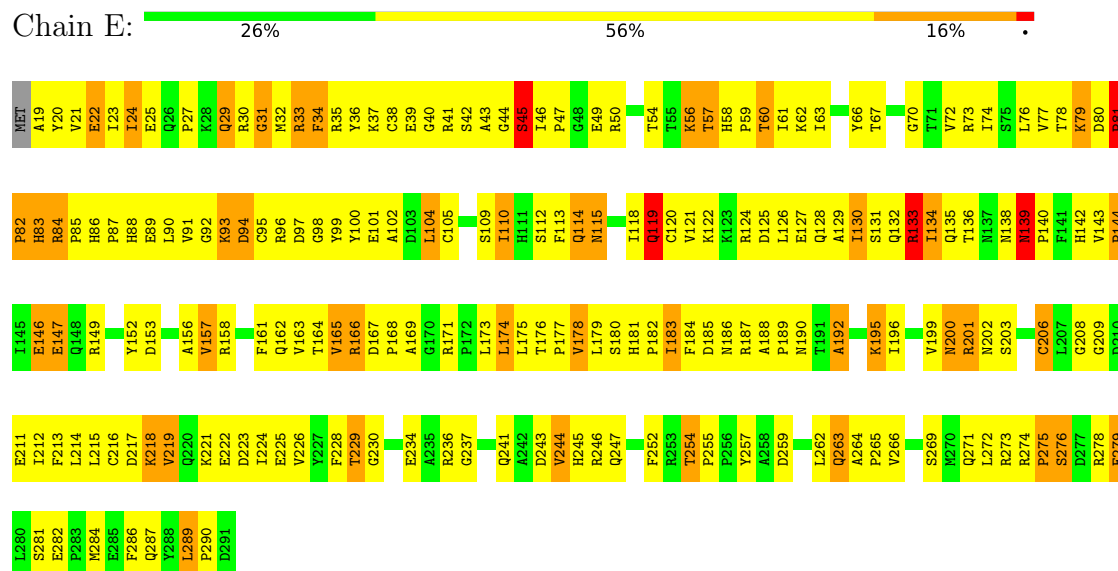
Chain	Residue	Modelled	Actual	Comment	Reference
B	38	MET	-	initiating methionine	UNP P25799
F	38	MET	-	initiating methionine	UNP P25799

Note EDS was not executed.

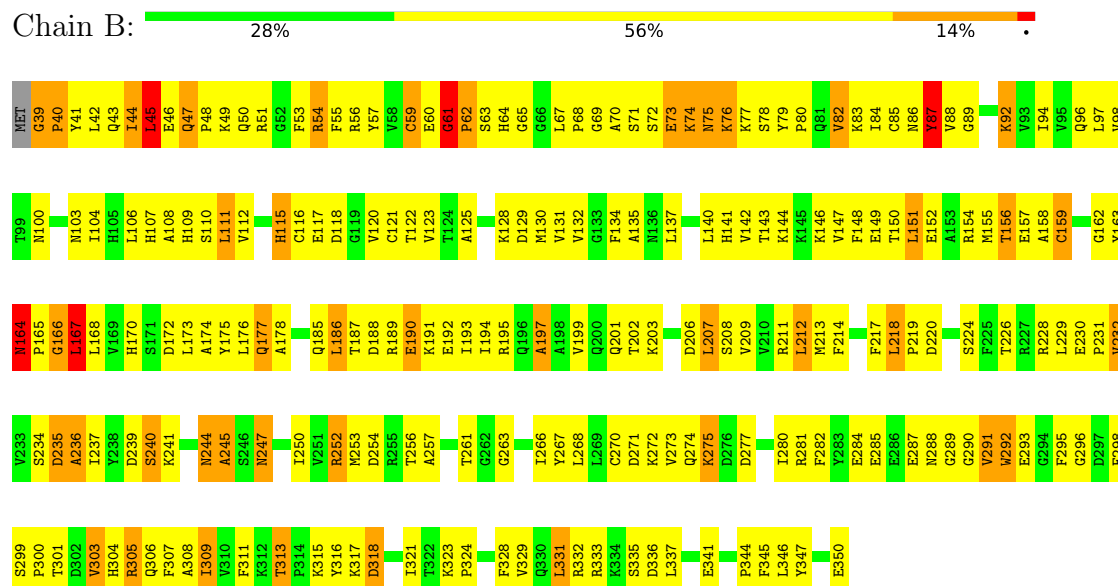
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|------|------|
| D80 | P81 | P82 | H83 | H84 | H85 | H86 | P87 | H88 | E89 | L90 | L91 | G92 | K93 | K94 | G95 | D96 | D97 | G98 | T99 | T100 | E101 | A102 | M103 | L104 | C105 | L106 | L107 | L108 | S109 | I110 | H111 | S112 | F113 | F114 | N115 | L116 | G117 | I118 | Q119 | C120 | M121 | K122 | K123 | R124 | D125 | L126 | F127 | Q128 | A129 | I130 | S131 | R132 | R133 | I134 | Q135 | T136 | N137 | N138 | M139 | T140 |
|------|------|



• Molecule 3: NUCLEAR FACTOR NF-KAPPA-B P65 SUBUNIT



• Molecule 4: NUCLEAR FACTOR NF-KAPPA-B P50 SUBUNIT



• Molecule 4: NUCLEAR FACTOR NF-KAPPA-B P50 SUBUNIT

Chain F: 30% 51% 17% .

MET	G39	P40	Y41	L42	Q43	I44	L45	E46	Q47	P48	K49	G101	K102	M103	I104	H105	L106	H107	A108	H109	S110	L111	V112	G113	K114	H115	C116	E117	D118	G119	V120	C121	T122	V123	L124	A125	G126	K127	K128	V131	V132	G133	F134	A135	N136	L137	G138	I139	L140	H141	V142	T143	K144	K145	K146	V147	F148	L151	E152	A153	R154	M155	T156	E157	A158	C159	I160	G162
												Y163	N164	P165	G166	L167	L168	V169	H170	S171	D172	L173	A174	V175	L176	Q177	A178	E179	G182	D183	R184	Q185	L186	T187	D188	R189	E190	K191	E192	I193	I194	R195	Q196	A197	V198	Q200	Q201	T202	M205	D206	L207	V210	R211	L212	M213	F214	T215	A216	F217	L218	P219	D220	S221	T222	G223	S224	F225	
												R228	L229	E230	S234	D235	A236	I237	Y238	D239	S240	K241	S246	N247	L248	K249	I250	M253	D254	V260	G263	Y267	L268	L269	C270	D271	K272	V273	Q274	K275	D276	D277	F282	Y283	E284	E285	E286	G290	V291	W292	E293	G294	F295	T301	D302	V303	H304	R305	Q306	F307	A308							
												I309	T313	P314	K315	K316	K317	D318	V319	N320	I321	T322	V327	F328	V329	R332	R333	K334	S335	D336	L337	E338	E341	F345	L346	P349	E350																															
												G39	P40	Y41	L42	Q43	I44	L45	E46	Q47	P48	K49	Q50	R51	G52	F53	R54	F55	R56	Y57	V58	C59	E60	G61	P62	S63	H64	G65	G66	L67	P68	S72	E73	K74	H75	G76	K77	S78	Y79	P80	Q81	V82	K83	I84	C85	N86	Y87	V88	A91	K92	V93	I94	V95	Q96	L97	V98	T99	N100

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.84Å 138.00Å 90.04Å 90.00° 97.28° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	85.4 (30.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.249 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10232	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality [i](#)

5.1 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 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	0.41	0/268	0.87	0/412
1	G	0.29	0/268	0.67	0/412
2	D	0.43	0/276	0.80	1/424 (0.2%)
2	H	0.26	0/276	0.48	0/424
3	A	0.54	0/2228	1.12	24/3021 (0.8%)
3	E	0.54	0/2228	1.09	15/3021 (0.5%)
4	B	0.54	0/2506	1.05	18/3384 (0.5%)
4	F	0.51	0/2506	1.02	19/3384 (0.6%)
All	All	0.52	0/10556	1.03	77/14482 (0.5%)

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
4	B	0	1

There are no bond length outliers.

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	80	ASP	CA-C-N	10.44	131.13	120.38
3	E	80	ASP	C-N-CA	10.44	131.13	120.38
3	A	119	GLN	OE1-CD-NE2	-9.79	112.81	122.60
3	E	119	GLN	OE1-CD-NE2	-9.77	112.83	122.60
3	A	80	ASP	N-CA-C	8.87	123.19	110.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	347	TYR	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	241	0	139	14	0
1	G	241	0	139	26	0
2	D	245	0	135	5	0
2	H	245	0	135	22	0
3	A	2176	0	2137	340	0
3	E	2176	0	2137	305	0
4	B	2454	0	2449	301	0
4	F	2454	0	2449	343	0
All	All	10232	0	9720	1301	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 65.

The worst 5 of 1301 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)
4:F:98:VAL:HG12	4:F:168:LEU:HD21	1.19	1.10
2:H:813:DA:H4'	2:H:814:DA:H5'	1.33	1.10
4:F:106:LEU:HD21	4:F:155:MET:HG2	1.38	1.03
4:B:143:THR:HG23	4:B:146:LYS:H	1.24	1.02
4:F:56:ARG:HA	4:F:56:ARG:HH11	1.23	1.00

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 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 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	271/274 (99%)	190 (70%)	55 (20%)	26 (10%)	0	2
3	E	271/274 (99%)	181 (67%)	68 (25%)	22 (8%)	1	3
4	B	310/313 (99%)	227 (73%)	61 (20%)	22 (7%)	1	4
4	F	310/313 (99%)	220 (71%)	61 (20%)	29 (9%)	0	2
All	All	1162/1174 (99%)	818 (70%)	245 (21%)	99 (8%)	0	3

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	45	SER
3	A	81	PRO
3	A	97	ASP
3	A	115	ASN
3	A	247	GLN

5.3.2 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 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	242/243 (100%)	212 (88%)	30 (12%)	4	20
3	E	242/243 (100%)	206 (85%)	36 (15%)	3	15
4	B	268/269 (100%)	239 (89%)	29 (11%)	6	26
4	F	268/269 (100%)	236 (88%)	32 (12%)	5	22
All	All	1020/1024 (100%)	893 (88%)	127 (12%)	4	20

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	331	LEU
4	F	142	VAL
3	E	130	ILE

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Mol	Chain	Res	Type
4	F	140	LEU
4	F	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	247	ASN
4	F	306	GLN
3	E	148	GLN
4	F	200	GLN
4	F	109	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.