



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 10, 2022 – 08:16 PM EST

PDB ID : 1LE5
Title : Crystal structure of a NF-kB heterodimer bound to an IFN γ -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

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 : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

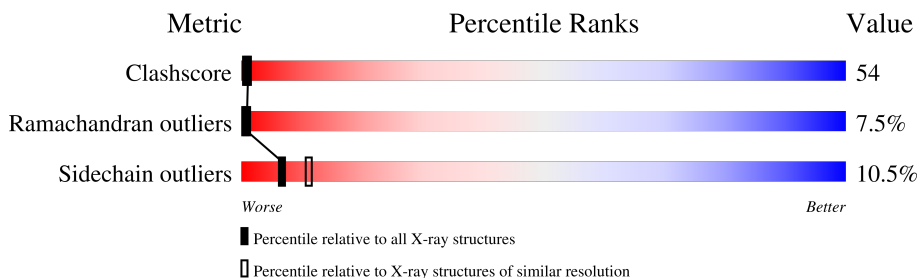
1 Overall quality at a glance

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	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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	50% 33% 17%
2	D	12	25% 75%
2	H	12	25% 8% 67%
3	A	274	31% 57% 12% .
3	E	274	31% 57% 10% .
4	B	313	28% 61% 10%
4	F	313	34% 52% 13% .

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 methionine	UNP P25799
F	38	MET	-	initiating methionine	UNP P25799

- Molecule 5 is water.

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

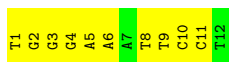
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: 



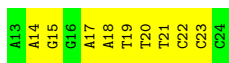
- Molecule 1: 5'-D(*TP*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*T)-3'

Chain G: 



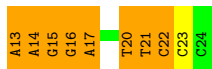
- Molecule 2: 5'-D(*AP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3'

Chain D: 




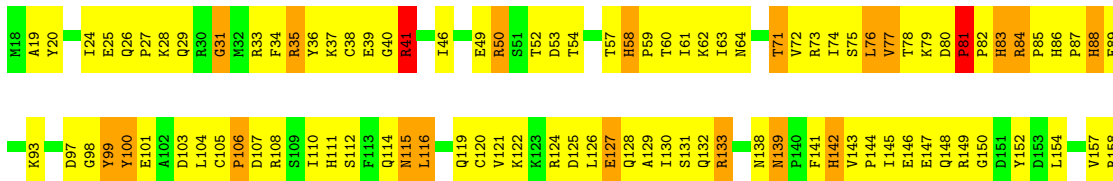
- Molecule 2: 5'-D(*AP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*C)-3'

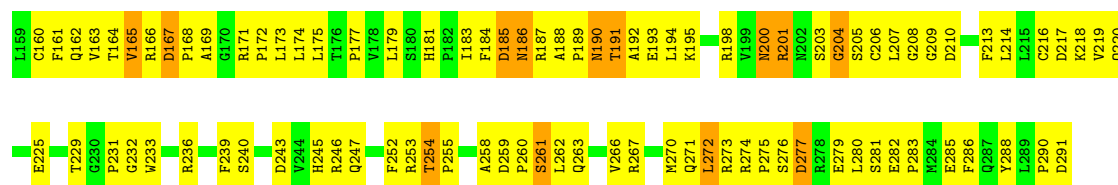
Chain H: 



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

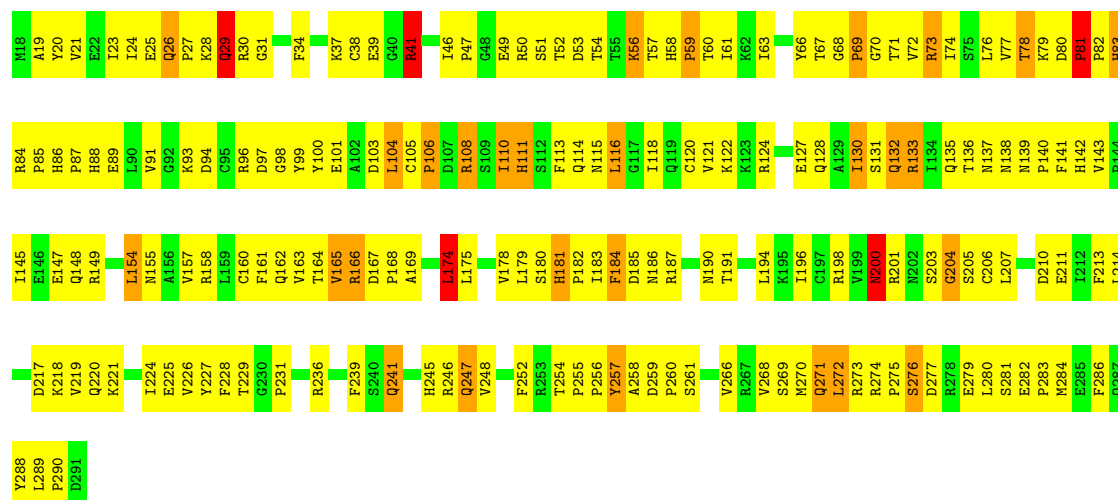
Chain A: 





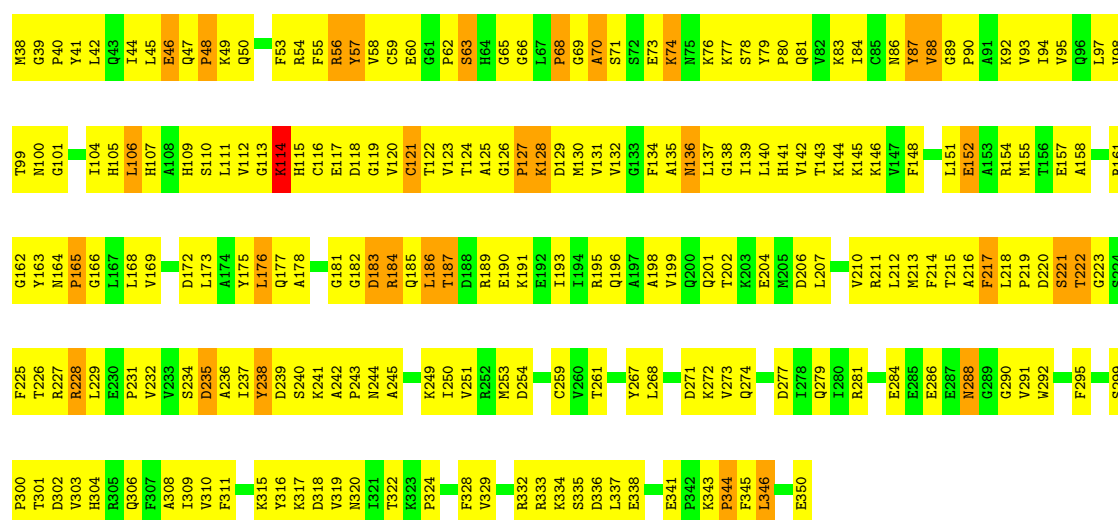
• Molecule 3: Nuclear factor NF-kappa-B p65 subunit

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%



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	137.53Å 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 ²)	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	1
3	E	272/274 (99%)	201 (74%)	50 (18%)	21 (8%)	1	0
4	B	311/313 (99%)	236 (76%)	54 (17%)	21 (7%)	1	1
4	F	311/313 (99%)	240 (77%)	44 (14%)	27 (9%)	1	0
All	All	1166/1174 (99%)	881 (76%)	197 (17%)	88 (8%)	1	0

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%)	7	12
3	E	243/243 (100%)	215 (88%)	28 (12%)	5	9
4	B	269/269 (100%)	244 (91%)	25 (9%)	9	15
4	F	269/269 (100%)	239 (89%)	30 (11%)	6	10
All	All	1024/1024 (100%)	916 (90%)	108 (10%)	7	11

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

Mol	Chain	Res	Type
3	E	81	PRO
3	E	236	ARG
4	F	227	ARG
3	E	104	LEU
3	E	154	LEU

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

Mol	Chain	Res	Type
3	E	29	GLN
3	E	186	ASN
4	F	247	ASN
3	E	111	HIS
3	E	138	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.