



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 05:08 PM UTC

PDB ID : 1NFI / pdb_00001nfi
Title : I-KAPPA-B-ALPHA/NF-KAPPA-B COMPLEX
Authors : Jacobs, M.D.; Harrison, S.C.
Deposited on : 1998-08-25
Resolution : 2.70 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

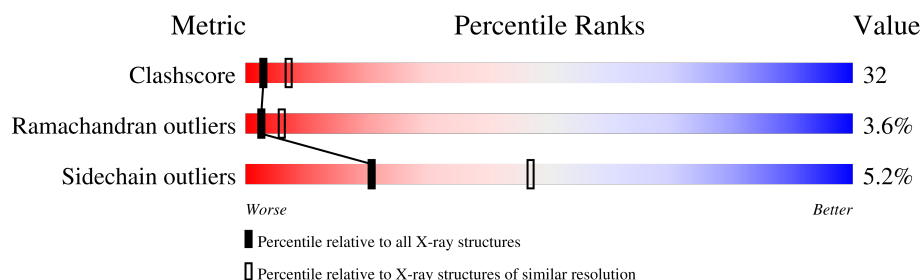
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	A	301	37% 52% 9% .
1	C	301	37% 55% 8%
2	B	107	72% 24% .
2	D	107	69% 26% 5%
3	E	213	59% 35% 7%
3	F	213	59% 36% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9890 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 protein called NF-KAPPA-B P65.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2380	1483	443	441	13			
1	C	301	Total	C	N	O	S	0	0	0
			2423	1511	450	449	13			

- Molecule 2 is a protein called NF-KAPPA-B P50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	107	Total	C	N	O	S	0	0	0
			875	562	145	165	3			
2	D	107	Total	C	N	O	S	0	0	0
			875	562	145	165	3			

- Molecule 3 is a protein called I-KAPPA-B-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1633	1026	287	311	9			
3	F	213	Total	C	N	O	S	0	0	0
			1633	1026	287	311	9			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	9	Total	O	0	0
			9	9		
4	C	11	Total	O	0	0
			11	11		
4	D	8	Total	O	0	0
			8	8		

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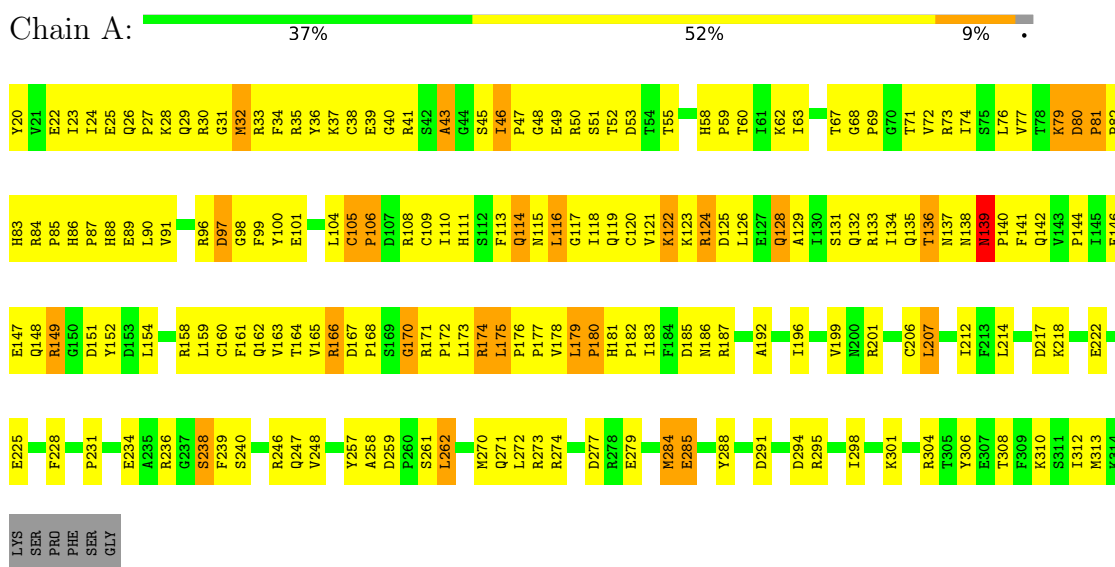
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	15	Total	O	0	0
			15	15		
4	F	17	Total	O	0	0
			17	17		

3 Residue-property plots

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.

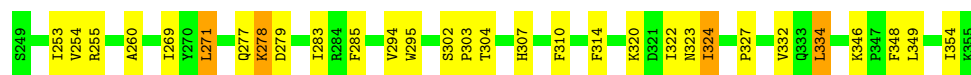
Note EDS was not executed.

• Molecule 1: NF-KAPPA-B P65



- Molecule 2: NF-KAPPA-B P50

Chain B:  72% 24% .



- Molecule 2: NF-KAPPA-B P50

Chain D:  69% 26% 5%



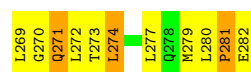
- Molecule 3: I-KAPPA-B-ALPHA

Chain E:  59% 35% 7%



- Molecule 3: I-KAPPA-B-ALPHA

Chain F:  59% 36% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.09 Å 91.08 Å 190.98 Å 90.00° 96.32° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	90.9 (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.223 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9890	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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	A	0.54	0/2436	1.11	18/3296 (0.5%)
1	C	0.56	0/2481	1.09	17/3356 (0.5%)
2	B	0.65	0/895	1.17	4/1207 (0.3%)
2	D	0.66	0/895	1.16	4/1207 (0.3%)
3	E	0.65	0/1663	1.14	14/2268 (0.6%)
3	F	0.62	0/1663	1.14	13/2268 (0.6%)
All	All	0.60	0/10033	1.12	70/13602 (0.5%)

There are no bond length outliers.

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	249	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	A	81	PRO	N-CA-C	9.80	122.65	110.70
3	E	249	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	C	81	PRO	N-CA-C	9.71	122.54	110.70
2	B	346	LYS	N-CA-C	-7.50	98.63	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	A	2380	0	2351	218	0
1	C	2423	0	2393	222	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	875	0	864	25	0
2	D	875	0	864	23	0
3	E	1633	0	1626	81	0
3	F	1633	0	1626	83	0
4	A	11	0	0	1	0
4	B	9	0	0	0	0
4	C	11	0	0	1	0
4	D	8	0	0	0	0
4	E	15	0	0	5	0
4	F	17	0	0	3	0
All	All	9890	0	9724	630	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 32.

The worst 5 of 630 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)
3:F:71:THR:HG22	3:F:72:GLU:H	1.11	1.10
3:E:254:TYR:HB2	3:E:272:LEU:HD21	1.42	1.01
3:F:254:TYR:HB2	3:F:272:LEU:HD21	1.43	0.99
1:A:310:LYS:HA	1:A:313:MET:HE2	1.42	0.99
1:A:159:LEU:O	1:A:180:PRO:HD3	1.64	0.97

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
1	A	293/301 (97%)	237 (81%)	42 (14%)	14 (5%)	2 3
1	C	299/301 (99%)	237 (79%)	48 (16%)	14 (5%)	2 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	105/107 (98%)	96 (91%)	7 (7%)	2 (2%)	6	17
2	D	105/107 (98%)	97 (92%)	6 (6%)	2 (2%)	6	17
3	E	211/213 (99%)	188 (89%)	17 (8%)	6 (3%)	4	9
3	F	211/213 (99%)	191 (90%)	14 (7%)	6 (3%)	4	9
All	All	1224/1242 (99%)	1046 (86%)	134 (11%)	44 (4%)	2	6

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ALA
1	A	97	ASP
1	A	114	GLN
1	A	137	ASN
1	A	174	ARG

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	
1	A	266/271 (98%)	248 (93%)	18 (7%)	14	35
1	C	271/271 (100%)	252 (93%)	19 (7%)	14	34
2	B	97/97 (100%)	95 (98%)	2 (2%)	47	75
2	D	97/97 (100%)	94 (97%)	3 (3%)	35	65
3	E	181/181 (100%)	174 (96%)	7 (4%)	28	57
3	F	181/181 (100%)	173 (96%)	8 (4%)	25	53
All	All	1093/1098 (100%)	1036 (95%)	57 (5%)	21	47

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	179	LEU
3	F	253	PRO

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Mol	Chain	Res	Type
1	C	262	LEU
3	F	245	ARG
3	F	78	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	96	GLN
3	F	105	ASN
3	F	188	HIS
1	C	29	GLN
1	C	26	GLN

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.