



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 07:52 am BST

PDB ID : 1NFK
Title : STRUCTURE OF THE NUCLEAR FACTOR KAPPA-B (NF-KB) P50 HOMODIMER
Authors : Ghosh, G.; Van Duyne, G.; Ghosh, S.; Sigler, P.B.
Deposited on : 1995-02-28
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (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) : 2.11

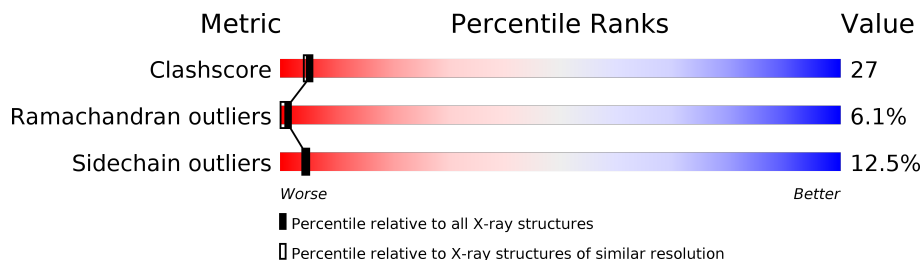
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 ≥ 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	11	45% 55%
1	D	11	64% 36%
2	A	325	52% 35% 7% . .
2	B	325	41% 45% 9% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7477 atoms, of which 1810 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 DNA (5'-D(*TP*GP*GP*GP*AP*AP*TP*TP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	11	Total	C	H	N	O	P	0	0	0
			246	107	24	40	65	10			
1	D	11	Total	C	H	N	O	P	0	0	0
			246	107	24	40	65	10			

- Molecule 2 is a protein called PROTEIN (NUCLEAR FACTOR KAPPA-B (NF-KB)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	312	Total	C	H	N	O	S	0	0	0
			3017	1554	564	428	459	12			
2	B	312	Total	C	H	N	O	S	0	0	0
			3017	1554	564	428	459	12			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	25	Total	H	O	0	0
			75	50	25		
3	D	26	Total	H	O	0	0
			78	52	26		
3	A	152	Total	H	O	0	0
			456	304	152		
3	B	114	Total	H	O	0	0
			342	228	114		

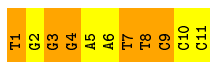
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

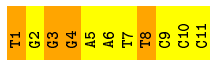
- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*AP*AP*TP*TP*CP*CP*C)-3')

Chain C: 



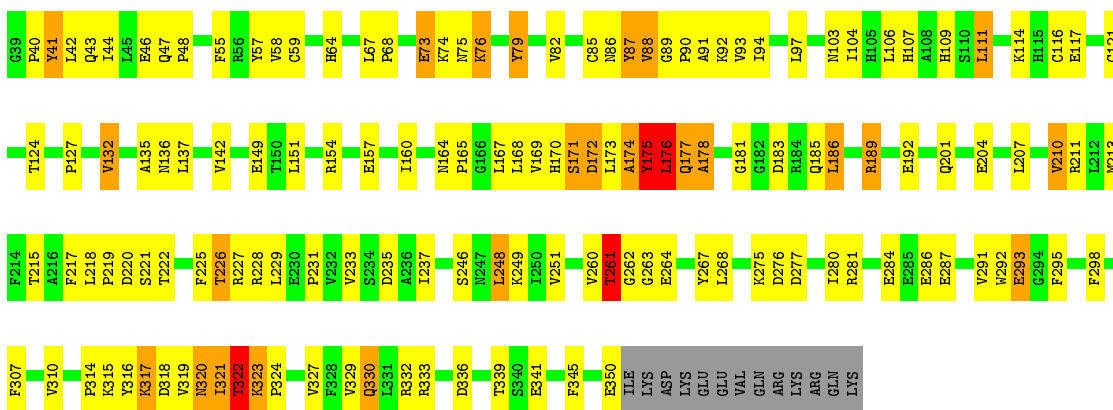
- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*AP*AP*TP*TP*CP*CP*C)-3')

Chain D: 



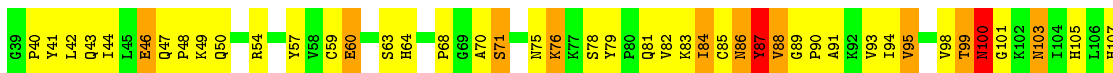
- Molecule 2: PROTEIN (NUCLEAR FACTOR KAPPA-B (NF-KB))

Chain A: 



- Molecule 2: PROTEIN (NUCLEAR FACTOR KAPPA-B (NF-KB))

Chain B: 



A108	H109	S110	L111	V112	G113	K114	H115	C116	G121	T122	V123	T124	A125	G126	V132	A135	M136	L137	G138	I139	L140	H141	V142	T143	K144	K145	K146	V147	F148	E149	T150	A153	R154	M155	T156	E157	A158	C159	L160	M164	P165	G166	L167	L168	D172	L173	A174	Y175	L176	Q177	A178	R184
Q185	L186	T187	D188	R189	E190	K191	E192	I193	I194	R195	Q196	V199	Q200	Q201	T202	K203	E204	M205	D206	L207	R211	L212	A216	F217	L218	P219	D220	S221	T222	G223	F225	S224	T226	R227	R228	L229	V232	V233	S234	D235	A236	S240	K241	L248	R252	M253	D254	R255	T256	V260	T261	
G262	G263	E264	E265	I266	Y267	L268	D276	I280	R281	F282	Y283	E284	E285	E286	E287	V291	W292	E293	G294	F295	G296	D297	F298	S299	P300	T301	R305	A308	F311	K312	K315	Y316	K317	D318	V319	N320	L321	T322	K323	S326	V327	F328	V329	R332	D336	L337	E338	T339				
P342	F345	L346	Y347	Y348	P349	E350	I1E	L1S	L1S	ASP	L1S	L1S	GLU	GLU	VAL	GLN	GLN	ARG	ARG	ARG	GLN	GLN	L1S																													

4 Data and refinement statistics

Xtrriage (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	84.20Å 132.10Å 80.10Å 90.00° 93.10° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.230 , 0.340	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7477	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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	2.99	26/248 (10.5%)	2.09	11/381 (2.9%)
1	D	3.47	38/248 (15.3%)	2.18	14/381 (3.7%)
2	A	0.60	0/2505	0.89	4/3384 (0.1%)
2	B	0.55	0/2505	0.84	3/3384 (0.1%)
All	All	1.12	64/5506 (1.2%)	1.06	32/7530 (0.4%)

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
2	A	0	1

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	7	DT	C5-C7	12.11	1.57	1.50
1	D	7	DT	C5'-C4'	-11.19	1.39	1.51
1	C	1	DT	N3-C4	-10.50	1.30	1.38
1	D	6	DA	N9-C4	10.27	1.44	1.37
1	C	8	DT	C5'-C4'	-9.51	1.40	1.51

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	DT	C4-C5-C7	-9.73	113.16	119.00
1	D	5	DA	O4'-C4'-C3'	-7.38	101.55	104.50
1	D	5	DA	O4'-C1'-N9	7.32	113.12	108.00
1	C	11	DC	O4'-C1'-N1	7.18	113.03	108.00
1	C	7	DT	C4-C5-C7	-6.69	114.98	119.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	175	TYR	Sidechain

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	C	222	24	125	5	0
1	D	222	24	126	7	0
2	A	2453	564	2449	121	0
2	B	2453	564	2451	152	0
3	A	152	304	0	10	0
3	B	114	228	0	4	0
3	C	25	50	0	1	0
3	D	26	52	0	2	0
All	All	5667	1810	5151	275	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 27.

The worst 5 of 275 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:9:DC:H2'	2:A:59:CYS:SG	1.97	1.05
1:C:1:DT:H2''	1:C:2:DG:H5'	1.42	0.99
2:B:218:LEU:HB2	2:B:227:ARG:HB3	1.41	0.99
2:A:92:LYS:HG2	2:A:124:THR:HG22	1.44	0.98
2:B:147:VAL:HG12	2:B:202:THR:HG22	1.54	0.89

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	
2	A	310/325 (95%)	257 (83%)	35 (11%)	18 (6%)	1	0
2	B	310/325 (95%)	251 (81%)	39 (13%)	20 (6%)	1	0
All	All	620/650 (95%)	508 (82%)	74 (12%)	38 (6%)	1	0

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	87	TYR
2	A	172	ASP
2	A	261	THR
2	A	317	LYS
2	A	322	THR

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	
2	A	268/281 (95%)	228 (85%)	40 (15%)	3	3
2	B	268/281 (95%)	241 (90%)	27 (10%)	7	9
All	All	536/562 (95%)	469 (88%)	67 (12%)	4	5

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	251	VAL

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Mol	Chain	Res	Type
2	A	332	ARG
2	B	256	THR
2	A	264	GLU
2	A	322	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	196	GLN
2	B	43	GLN
2	B	136	ASN
2	A	164	ASN
2	B	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 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 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.