



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:01 AM UTC

PDB ID : 1VKX / pdb_00001vkx
Title : CRYSTAL STRUCTURE OF THE NFKB P50/P65 HETERODIMER COM-
PLEXED TO THE IMMUNOGLOBULIN KB DNA
Authors : Chen, F.; Huang, D.B.; Ghosh, G.
Deposited on : 1997-09-17
Resolution : 2.90 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

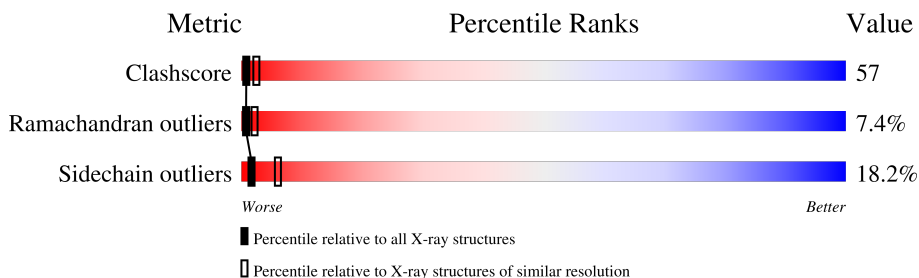
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	
2	D	12	
3	A	273	
4	B	312	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5116 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 DNA (5'-D(*TP*GP*GP*GP*GP*AP*CP*TP*TP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			243	117	42	73	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			243	116	49	67	11			

- Molecule 3 is a protein called PROTEIN (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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	PRO	conflict	UNP Q04207

- Molecule 4 is a protein called PROTEIN (NF-KAPPA B P50 SUBUNIT).

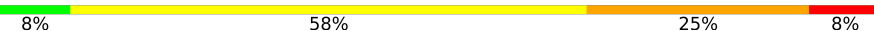
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	312	Total	C	N	O	S	0	0	0
			2454	1554	428	460	12			

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.

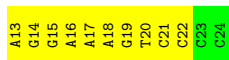
- Molecule 1: DNA (5'-D(*TP*GP*GP*GP*GP*AP*CP*TP*TP*TP*CP*C)-3')

Chain C: 

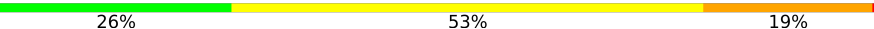


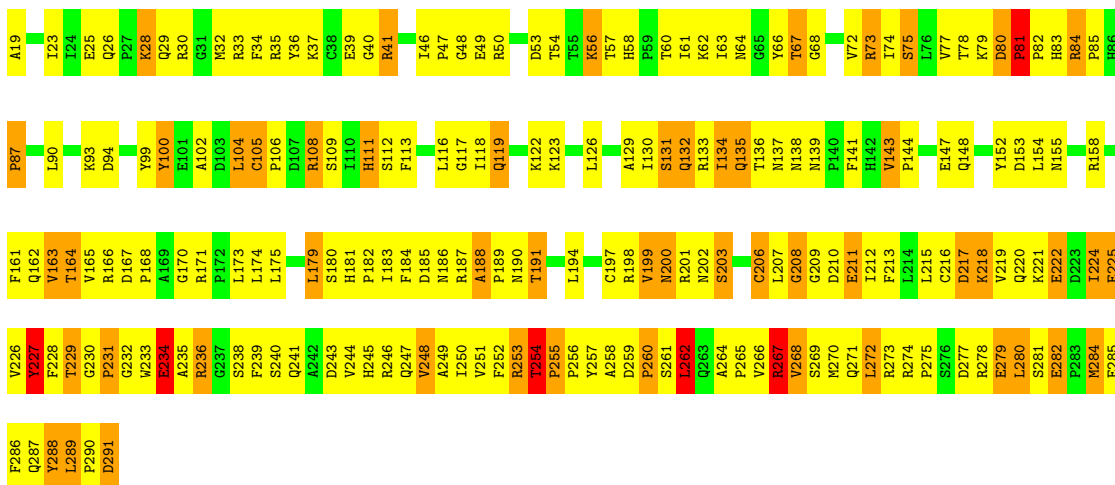
- Molecule 2: DNA (5'-D(*AP*GP*GP*AP*AP*AP*GP*TP*CP*CP*CP*C)-3')

Chain D: 

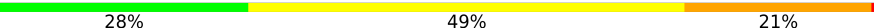


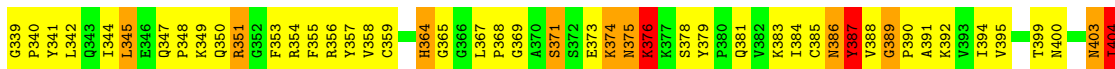
- Molecule 3: PROTEIN (NF-KAPPA B P65 SUBUNIT)

Chain A: 



- Molecule 4: PROTEIN (NF-KAPPA B P50 SUBUNIT)

Chain B: 



H405	L473	Y538	T601	H406	A474	D539	D602	H407	Y475	S540	V603	H408	L476	K541	H604	R605	Q606	F607	A489	Q477	F543	N544	A480	S546	N547	F611	K612	T613	P614	K615	Y616	K617	D618	V619	M620	I621	T622	K623	P624	A625	S626	V627	F628	V629	Q630	L631	R632	R633	A634	S635	D636	L637	E638	T639	S640	E641	L646	Y647	Y648	P649	E650															
H409	A478	K542	R606	A488	Y479	M553	F608	A490	Q481	I550	V604	A491	Q482	L548	H605	G590	V591	W592	E593	G594	F595	G596	D597	F598	S599	P600	D601	K614	P615	K616	Y617	D619	M621	T623	K624	P625	S627	V628	F629	Q631	L632	R634	A635	D637	L638	E639	T640	S641	E642	L647	Y649	P650	E651	L648	Y650	F651	G652	H653	I654	J655	K656	L657	M658	N659	O660	P661	Q662	R663	S664	T665	U666	V667	W668	X669	Y670	Z671

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.61Å 106.61Å 206.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.208 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5116	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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	0.57	0/271	1.05	2/417 (0.5%)
2	D	0.52	0/273	0.82	0/419
3	A	0.85	2/2228 (0.1%)	1.47	41/3021 (1.4%)
4	B	0.82	1/2506 (0.0%)	1.32	33/3384 (1.0%)
All	All	0.81	3/5278 (0.1%)	1.35	76/7241 (1.0%)

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	C	0	3
3	A	0	1
4	B	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	118	ILE	C-N	-7.57	1.22	1.33
4	B	639	THR	CA-C	-6.19	1.50	1.53
3	A	119	GLN	C-N	-5.15	1.25	1.33

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	135	GLN	N-CA-C	-12.13	95.59	111.24
3	A	81	PRO	CA-C-N	-11.17	106.27	120.79
3	A	81	PRO	C-N-CA	-11.17	106.27	120.79
3	A	254	THR	CA-C-N	10.67	127.45	119.66
3	A	254	THR	C-N-CA	10.67	127.45	119.66

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	227	TYR	Sidechain
4	B	387	TYR	Sidechain
1	C	1	DT	Sidechain
1	C	3	DG	Sidechain
1	C	9	DT	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	243	0	138	40	0
2	D	243	0	135	37	0
3	A	2176	0	2137	232	0
4	B	2454	0	2449	288	0
All	All	5116	0	4859	570	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 57.

The worst 5 of 570 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)
2:D:19:DG:C8	2:D:20:DT:H72	1.77	1.18
4:B:487:THR:HB	4:B:490:GLU:HB2	1.26	1.17
2:D:13:DA:H2''	2:D:14:DG:H5''	1.22	1.16
1:C:2:DG:H2''	1:C:3:DG:C5'	1.82	1.10
4:B:465:PRO:HB2	4:B:467:LEU:HD13	1.32	1.08

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	271/273 (99%)	208 (77%)	44 (16%)	19 (7%)	1	2
4	B	310/312 (99%)	241 (78%)	45 (14%)	24 (8%)	1	2
All	All	581/585 (99%)	449 (77%)	89 (15%)	43 (7%)	1	2

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	29	GLN
3	A	40	GLY
3	A	81	PRO
3	A	209	GLY
3	A	231	PRO

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	242/242 (100%)	191 (79%)	51 (21%)	1	4
4	B	268/268 (100%)	226 (84%)	42 (16%)	2	9
All	All	510/510 (100%)	417 (82%)	93 (18%)	2	6

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	403	ASN

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Mol	Chain	Res	Type
4	B	500	GLN
4	B	420	VAL
4	B	475	TYR
4	B	529	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	409	HIS
4	B	501	GLN
4	B	500	GLN
4	B	544	ASN
3	A	220	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.