



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2021 – 06:11 PM JST

PDB ID : 7VUP  
Title : Structure of NF-kB p52 homodimer bound to +1/-1 swap P-Selectin kB DNA fragment  
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Deposited on : 2021-11-04  
Resolution : 3.40 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

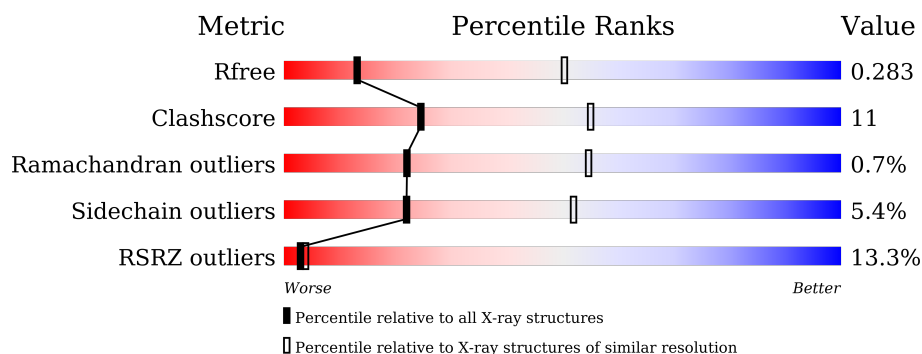
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	398	
1	B	398	
2	C	18	
3	D	18	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5359 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 Nuclear factor NF-kappa-B p52 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2334	1469	420	433	12			
1	B	296	Total	C	N	O	S	0	0	0
			2334	1469	420	433	12			

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*AP\*AP\*GP\*GP\*GP\*GP\*AP\*CP\*TP\*CP\*CP\*CP\*CP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	P	0	0	0
			341	163	62	100	16			

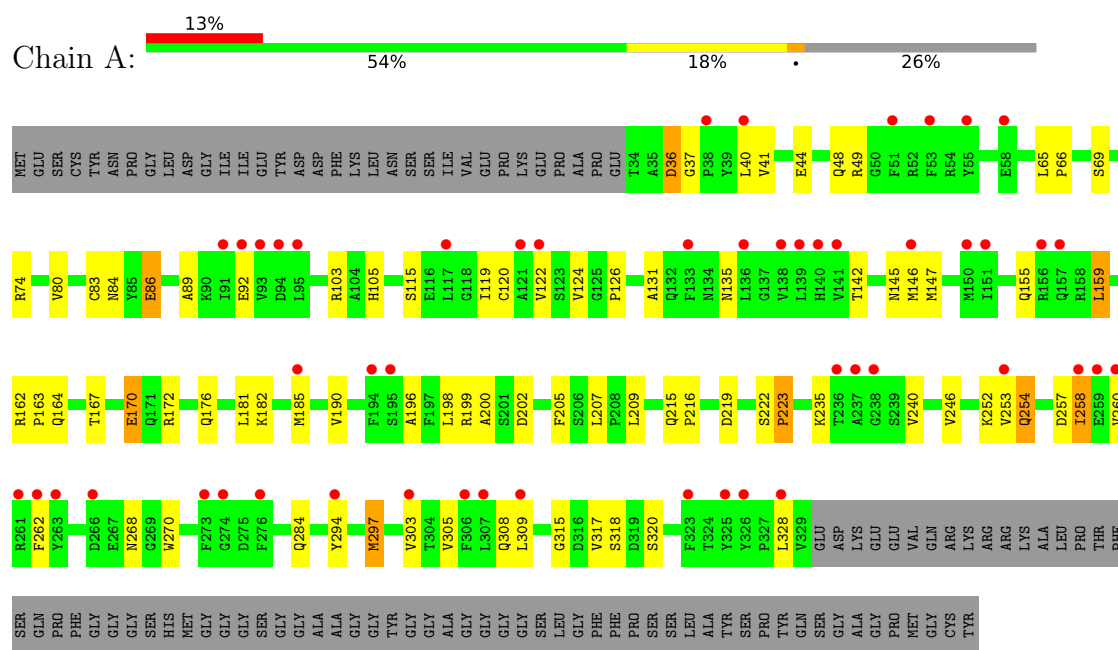
- Molecule 3 is a DNA chain called DNA (5'-D(\*AP\*AP\*GP\*GP\*GP\*GP\*GP\*AP\*GP\*TP\*CP\*CP\*CP\*CP\*TP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	17	Total	C	N	O	P	0	0	0
			350	166	68	100	16			

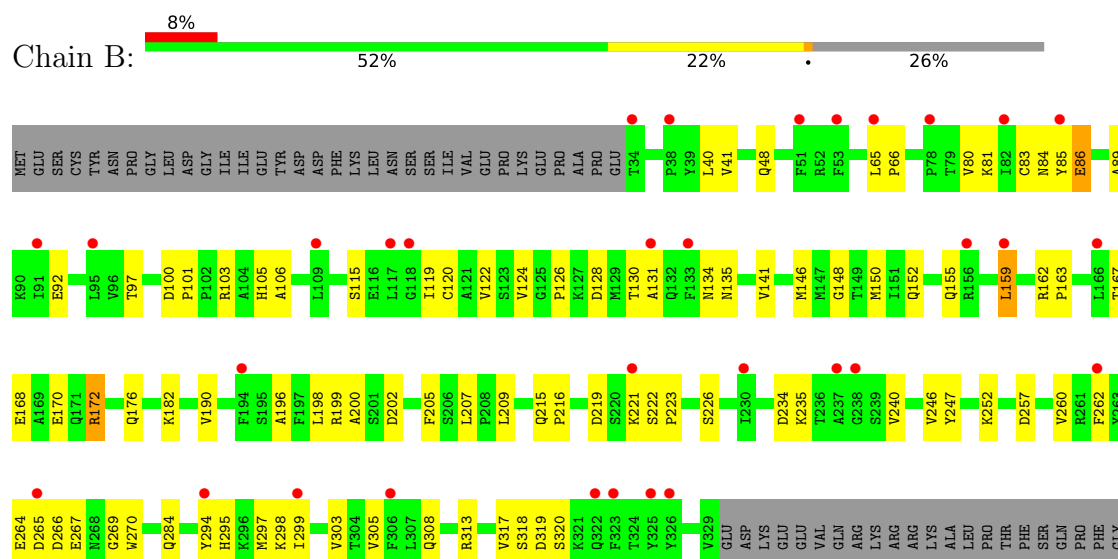
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

#### • Molecule 1: Nuclear factor NF-kappa-B p52 subunit

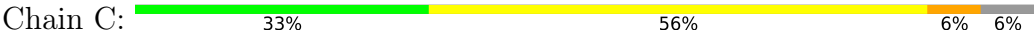


#### • Molecule 1: Nuclear factor NF-kappa-B p52 subunit



GLY	GLY	SER	HIS	MET	GLY	GLY	GLY	SER	GLY	GLY	ALA	ALA	GLY	GLY	TYR	GLY	GLY	ALA	GLY	GLY	GLY	SER	LEU	GLY	PHE	PRO	SER	SER	LEU	ALA	TYR	SER	PRO	TYR	GLN	SER	GLY	ALA	GLY	PRO	MET	GLY	CYS	TYR
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● Molecule 2: DNA (5'-D(\*CP\*AP\*AP\*GP\*GP\*GP\*GP\*AP\*CP\*TP\*CP\*CP\*CP\*CP\*TP\*T)-3')



C1	A2	A3	C4	G5	G6	G7	A8	C9	T10	C11	C12	C13	C14	C15	T16	T17	DC
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● Molecule 3: DNA (5'-D(\*AP\*AP\*GP\*GP\*GP\*GP\*GP\*AP\*GP\*TP\*CP\*CP\*CP\*CP\*TP\*TP\*G)-3')



DC	A2	A3	C4	G5	G8	A9	C12	C13	C14	C15	T16	T17	G18
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.99Å 84.29Å 140.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.45 – 3.40 45.41 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.45-3.40) 99.7 (45.41-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.271 , 0.286 0.271 , 0.283	Depositor DCC
$R_{free}$ test set	690 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	118.0	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 108.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.045 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5359	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1259e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	A	0.66	0/2384	0.86	0/3211
1	B	0.65	0/2384	0.86	0/3211
2	C	0.92	0/381	1.45	6/585 (1.0%)
3	D	0.95	0/393	1.44	3/606 (0.5%)
All	All	0.70	0/5542	0.97	9/7613 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	DA	P-O3'-C3'	-12.41	104.81	119.70
2	C	5	DG	P-O3'-C3'	-8.39	109.63	119.70
3	D	9	DA	P-O3'-C3'	-6.88	111.44	119.70
3	D	8	DG	P-O3'-C3'	-6.34	112.09	119.70
2	C	4	DG	P-O3'-C3'	-5.93	112.58	119.70

There are no chirality outliers.

There are no planarity outliers.

### 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	A	2334	0	2345	48	2
1	B	2334	0	2345	57	2
2	C	341	0	192	7	0
3	D	350	0	192	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5359	0	5074	113	2

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 11.

The worst 5 of 113 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:A:44:GLU:OE2	1:A:69:SER:OG	1.64	1.14
1:B:40:LEU:HD12	1:B:196:ALA:HB2	1.52	0.90
1:A:40:LEU:HD12	1:A:196:ALA:HB2	1.53	0.90
1:B:40:LEU:HD21	1:B:80:VAL:HB	1.56	0.88
1:A:40:LEU:HD21	1:A:80:VAL:HB	1.57	0.85

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:NH2	1:B:128:ASP:OD1[2_455]	1.65	0.55
1:A:74:ARG:NH2	1:B:128:ASP:CG[2_455]	2.13	0.07

## 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	294/398 (74%)	270 (92%)	21 (7%)	3 (1%)	15	46
1	B	294/398 (74%)	280 (95%)	13 (4%)	1 (0%)	41	72
All	All	588/796 (74%)	550 (94%)	34 (6%)	4 (1%)	22	55

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	36	ASP
1	B	85	TYR
1	A	223	PRO
1	A	315	GLY

### 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	257/330 (78%)	244 (95%)	13 (5%)	24	54
1	B	257/330 (78%)	242 (94%)	15 (6%)	20	50
All	All	514/660 (78%)	486 (95%)	28 (5%)	22	52

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	134	ASN
1	B	320	SER
1	B	172	ARG
1	B	298	LYS
1	B	168	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	ASN
1	B	134	ASN
1	B	145	ASN
1	B	282	HIS
1	B	295	HIS

### 5.3.3 RNA ⓘ

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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	296/398 (74%)	0.73	51 (17%) <b>1</b> <b>1</b>	110, 160, 240, 289	0
1	B	296/398 (74%)	0.67	32 (10%) <b>5</b> <b>7</b>	102, 156, 229, 282	0
2	C	17/18 (94%)	0.10	0 <b>100</b> <b>100</b>	142, 169, 213, 228	0
3	D	17/18 (94%)	0.28	0 <b>100</b> <b>100</b>	146, 172, 212, 230	0
All	All	626/832 (75%)	0.67	83 (13%) <b>3</b> <b>4</b>	102, 160, 234, 289	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	GLY	5.6
1	A	260	VAL	5.2
1	B	322	GLN	4.8
1	A	325	TYR	4.7
1	A	262	PHE	4.6

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.