



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:04 AM UTC

PDB ID : 1RAM / pdb\_00001ram  
Title : A NOVEL DNA RECOGNITION MODE BY NF-KB P65 HOMODIMER  
Authors : Chen, Y.-Q.; Ghosh, S.; Ghosh, G.  
Deposited on : 1997-11-22  
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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

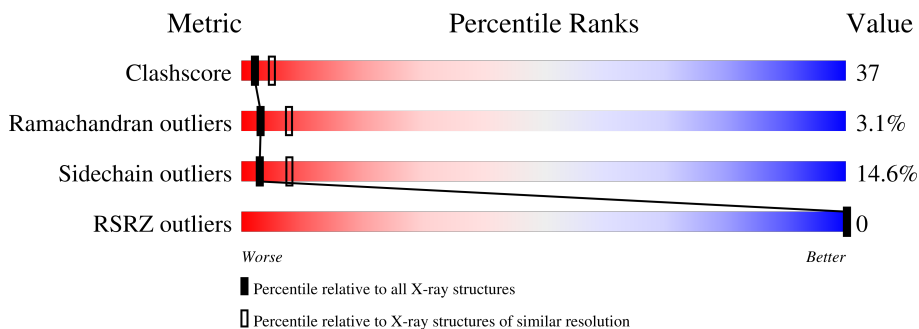
# 1 Overall quality at a glance

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)
RSRZ outliers	180081	3538 (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  $\geq 3$ , 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	C	20	5% <span style="float: right;">95%</span>
1	D	20	50% <span style="float: right;">50%</span>
2	A	273	48% <span style="float: right;">38%</span> 12% <span style="float: right;">•</span>
2	B	273	42% <span style="float: right;">45%</span> 12% <span style="float: right;">•</span>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DTT	A	1	X	-	-	-
3	DTT	B	2	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5202 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.

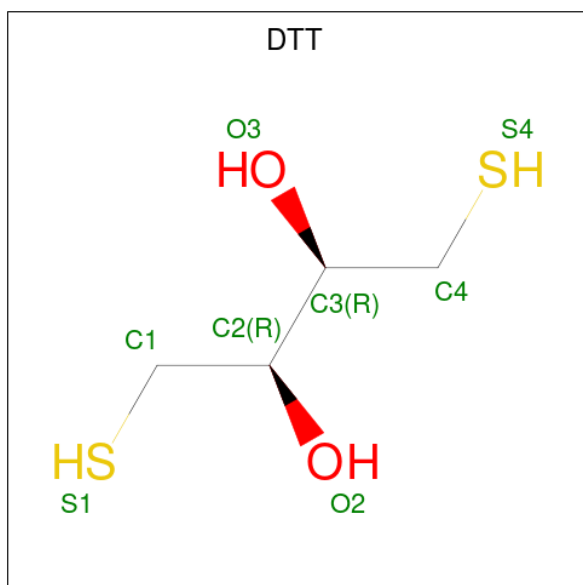
- Molecule 1 is a DNA chain called DNA (5'-D(\*CP\*GP\*GP\*CP\*TP\*GP\*GP\*AP\*AP\*AP\*TP\*TP\*TP\*CP\*CP\*AP\*GP\*CP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	20	Total 407	C 194	N 76	O 118	P 19	0	0	0
1	D	20	Total 407	C 194	N 76	O 118	P 19	0	0	0

- Molecule 2 is a protein called PROTEIN (TRANSCRIPTION FACTOR NF-KB P65).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	273	Total 2178	C 1358	N 401	O 408	S 11	0	0	0
2	B	273	Total 2178	C 1358	N 401	O 408	S 11	0	0	0

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		
3	B	1	Total	C	O	S	0	0
			8	4	2	2		

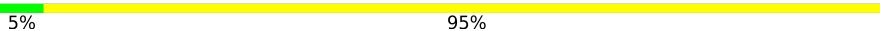
- Molecule 4 is water.

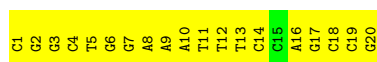
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total	O	0	0
			3	3		
4	D	2	Total	O	0	0
			2	2		
4	A	5	Total	O	0	0
			5	5		
4	B	6	Total	O	0	0
			6	6		

### 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 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.

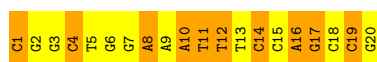
- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*CP\*TP\*GP\*GP\*AP\*AP\*AP\*TP\*TP\*TP\*CP\*CP\*AP\*GP\*CP\*CP\*G)-3')

Chain C:  5% 95%



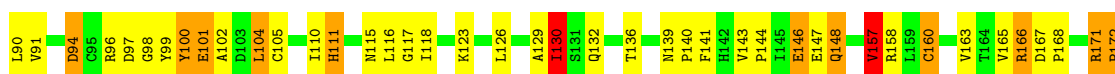
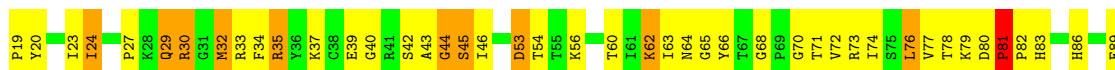
- Molecule 1: DNA (5'-D(\*CP\*GP\*GP\*CP\*TP\*GP\*GP\*AP\*AP\*AP\*TP\*TP\*TP\*CP\*CP\*AP\*GP\*CP\*CP\*G)-3')

Chain D:  50% 50%



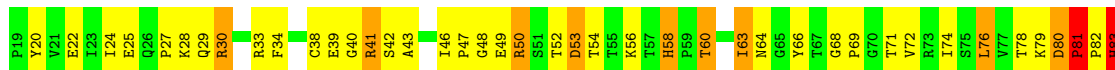
- Molecule 2: PROTEIN (TRANSCRIPTION FACTOR NF-KB P65)

Chain A:  48% 38% 12%



- Molecule 2: PROTEIN (TRANSCRIPTION FACTOR NF-KB P65)

Chain B:  42% 45% 12%



R84	P85	H86	P87	H88	E89	L90	K93	D94	C95	R96	D97	G98	Y99	Y100	E101	A102	D103	L104	C105	P106	D107	R108	S109	L110	H111	S112	F113	Q114	N115	L116	G117	C120	V121	K122	D125	L126	E127	Q128	R133	L134	Q135	T136	N137	M138	M139	P140	F141	H142	V143	P144	L145	E146	E147	Q148	R149
G150	D151	Y152	D153	L154	M155	R158	L159	C160	F161	Q162	V163	R166	R171	L175	L179	S180	H181	P182	I183	F184	D185	M186	R187	A188	P189	M190	T191	L194	K195	I196	C197	R198	R201	N202	S203	G204	S205	C206	L207	L214	D217	K218	V219	Q220	Q221	F222	D223	L224	E225	V226					
Y227	F228	T229	W233	E234	A235	R236	F239	S240	Q241	H245	R246	Q247	V248	F252	R253	T254	Y257	A258	L262	V266	R267	V268	S269	M270	Q271	L272	R273	R274	P275	R278	E279	L280	S281	L289	P290	D291																			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.69Å 81.08Å 167.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.2 (6.00-2.70) 87.4 (6.00-2.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.51Å)	Xtrriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.222 , 0.324 0.229 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.2	Xtrriage
Anisotropy	0.357	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 103.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DTT

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	0.51	0/456	0.89	0/702
1	D	0.55	0/456	1.23	6/702 (0.9%)
2	A	0.80	0/2231	1.26	23/3025 (0.8%)
2	B	0.69	0/2231	1.24	22/3025 (0.7%)
All	All	0.72	0/5374	1.22	51/7454 (0.7%)

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	1
1	D	0	5
2	B	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	80	ASP	CA-C-N	12.95	133.72	120.38
2	B	80	ASP	C-N-CA	12.95	133.72	120.38
2	B	81	PRO	N-CA-C	10.67	123.72	110.70
2	A	81	PRO	N-CA-C	8.85	121.50	110.70
2	A	183	ILE	N-CA-C	-8.57	96.17	108.17

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	14	DC	Sidechain
1	D	10	DA	Sidechain
1	D	14	DC	Sidechain
1	D	17	DG	Sidechain
1	D	4	DC	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	407	0	226	56	0
1	D	407	0	226	57	0
2	A	2178	0	2140	116	0
2	B	2178	0	2140	154	0
3	A	8	0	10	0	0
3	B	8	0	10	3	0
4	A	5	0	0	0	0
4	B	6	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	1	0
All	All	5202	0	4752	356	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 37.

The worst 5 of 356 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:D:1:DC:H5'	1:D:2:DG:C8	1.78	1.19
1:C:8:DA:H2''	1:C:9:DA:C5'	1.79	1.11
1:D:1:DC:H5'	1:D:2:DG:H8	1.10	1.09
1:C:8:DA:H2''	1:C:9:DA:H5'	1.31	1.08
2:B:89:GLU:HG2	2:B:133:ARG:HH22	1.19	1.07

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	271/273 (99%)	234 (86%)	28 (10%)	9 (3%)	3	7
2	B	271/273 (99%)	227 (84%)	36 (13%)	8 (3%)	3	8
All	All	542/546 (99%)	461 (85%)	64 (12%)	17 (3%)	3	8

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	44	GLY
2	A	45	SER
2	A	81	PRO
2	B	81	PRO
2	B	83	HIS

### 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	243/243 (100%)	201 (83%)	42 (17%)	2	5
2	B	243/243 (100%)	214 (88%)	29 (12%)	5	13
All	All	486/486 (100%)	415 (85%)	71 (15%)	3	8

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	135	GLN

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Mol	Chain	Res	Type
2	B	149	ARG
2	B	190	ASN
2	A	168	PRO
2	A	167	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	115	ASN
2	B	132	GLN
2	B	287	GLN
2	B	220	GLN
2	B	241	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DTT	B	2	-	7,7,7	0.61	0	4,8,8	0.41	0
3	DTT	A	1	-	7,7,7	0.94	0	4,8,8	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTT	B	2	-	2/2/2/2	1/8/8/8	-
3	DTT	A	1	-	2/2/2/2	4/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1	DTT	C2
3	A	1	DTT	C3
3	B	2	DTT	C2
3	B	2	DTT	C3

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	DTT	C1-C2-C3-O3
3	A	1	DTT	C1-C2-C3-C4
3	A	1	DTT	O2-C2-C3-O3
3	A	1	DTT	O2-C2-C3-C4
3	B	2	DTT	O3-C3-C4-S4

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	DTT	3	0

## 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	C	20/20 (100%)	-0.47	0 100 100	25, 51, 83, 84	0
1	D	20/20 (100%)	-0.36	0 100 100	20, 43, 74, 85	0
2	A	273/273 (100%)	-0.85	0 100 100	14, 37, 64, 87	0
2	B	273/273 (100%)	-0.58	0 100 100	16, 48, 87, 100	0
All	All	586/586 (100%)	-0.69	0 100 100	14, 42, 75, 100	0

There are no RSRZ outliers to report.

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	DTT	B	2	8/8	0.84	0.11	75,80,83,91	0
3	DTT	A	1	8/8	0.96	0.09	39,64,80,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.