W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 07:48 am BST

PDB ID	:	3JV4
Title	:	Crystal structure of the dimerization domains p50 and RelB
Authors	:	Vu, D.; Huang, D.B.; Ghosh, G.
Deposited on	:	2009-09-15
Resolution	:	3.15 Å(reported)

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	:	2.11
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)	:	2.11

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 3.15 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.
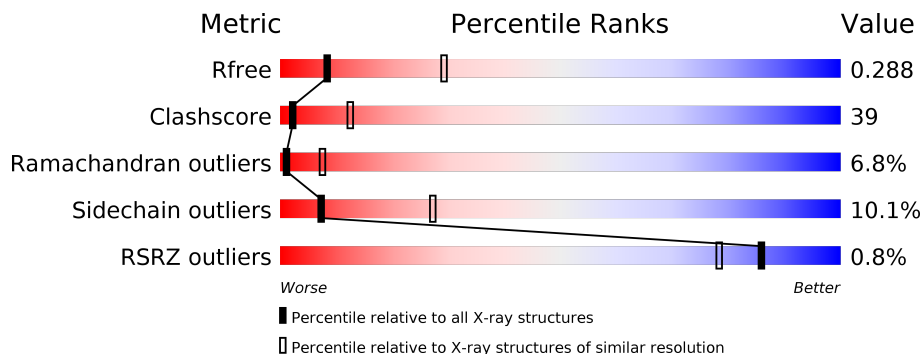
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 <=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	101	2% / 38% 52% 9% •
1	C	101	% / 36% 55% 9%
1	E	101	% / 38% 53% 9%
2	B	115	33% 56% 9% •
2	D	115	43% 46% 10% •
2	F	115	% / 37% 53% 7% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5185 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 Transcription factor RelB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			800	507	132	157	4			
1	C	101	Total	C	N	O	S	0	0	0
			800	507	132	157	4			
1	E	101	Total	C	N	O	S	0	0	0
			800	507	132	157	4			

- Molecule 2 is a protein called Nuclear factor NF-kappa-B p105 subunit.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	115	Total	C	N	O	S	0	0	0
			932	594	154	181	3			
2	D	115	Total	C	N	O	S	0	0	0
			942	600	158	181	3			
2	F	112	Total	C	N	O	S	0	0	0
			911	581	150	177	3			

3 Residue-property plots ⓘ

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 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.
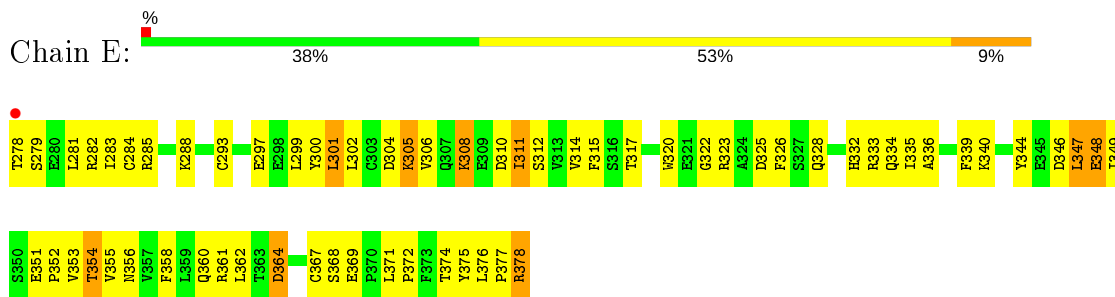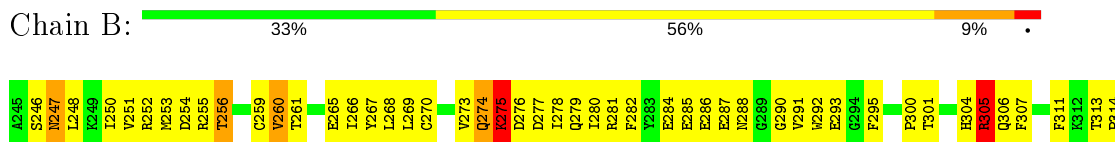
- Molecule 1: Transcription factor RelB
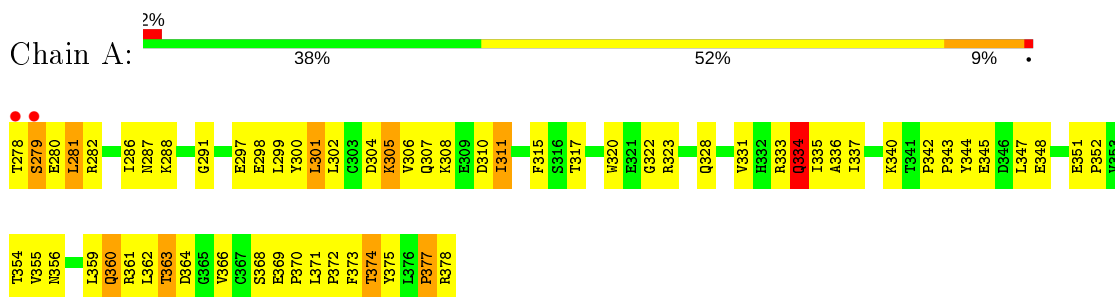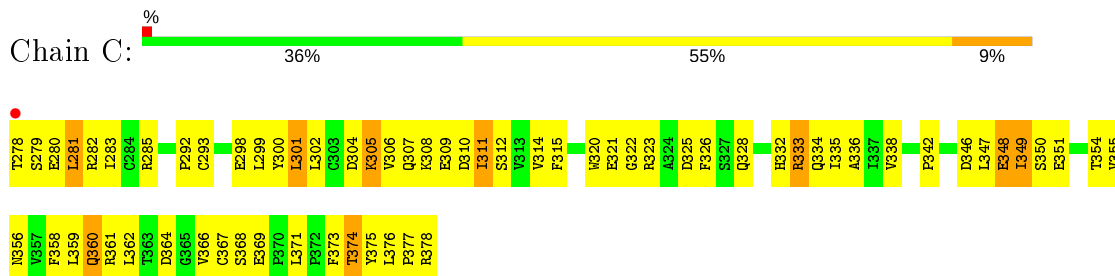
Chain A:

- Molecule 1: Transcription factor RelB
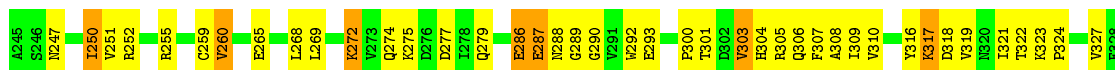
Chain C:

- Molecule 1: Transcription factor RelB

Chain E:

- Molecule 2: Nuclear factor NF-kappa-B p105 subunit

Chain B:

K315 Y316 K317 D318 V319 N320 I321 T322 K323 V327 L331 R332 R333 K334 S335 D336 L337 S340 E341 P342 P349 E350 I351 K352 D353 K354 E355 E356 V357 Q358 R359

• Molecule 2: Nuclear factor NF-kappa-B p105 subunit

Chain D:

43%   46%   10%   •

A245 S246 N247 I250 V251 R252 R255 C259 V260 E265 L268 L269 K272 V273 Q274 K275 D276 D277 I278 Q279 E286 E287 N288 G289 G290 V291 W292 E293 P300 T301 D302 V303 H304 R305 Q306 F307 A308 I309 V310 Y316 K317 D318 V319 N320 I321 T322 K323 P324 V327 F328

V329 Q330 L331 R332 R333 K334 S335 D336 L337 E338 T339 S340 E341 P342 K343 P344 F345 L346 Y347 Y348 P349 E350 I351 K352 D353 A354 E355 E356 V357 Q358 R359

• Molecule 2: Nuclear factor NF-kappa-B p105 subunit

Chain F:

%
37%   53%   7%   ••

A245 L248 K249 I250 V251 R252 M253 D254 R255 V260 T261 G262 Y267 L268 L269 C270 D271 K272 V273 Q274 K275 D276 D277 I278 Q279 I280 R281 F282 E285 E286 E287 N288 G289 G290 V291 W292 E293 G294 F295 G296 D297 F298 V303 H304 R305 Q306 F307 A308 I309 V310 F311 K312 T313 F314 K315

Y316 K317 D318 V319 N320 I321 P324 Q330 L331 R332 R333 K334 S335 D336 L337 E338 T339 S340 K343 P344 F345 L346 Y347 Y348 P349 E356 E356 VAL GLN ARG

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.17Å 106.17Å 143.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.76 – 3.15 42.50 – 3.14	Depositor EDS
% Data completeness (in resolution range)	81.6 (29.76-3.15) 90.7 (42.50-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.280 0.231 , 0.288	Depositor DCC
R_{free} test set	792 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	83.3	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 45.2	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5185	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.39	0/817	0.67	0/1111
1	C	0.43	0/817	0.72	0/1111
1	E	0.35	0/817	0.62	0/1111
2	B	0.49	0/952	0.75	1/1285 (0.1%)
2	D	0.48	0/962	0.75	0/1296
2	F	0.44	0/931	0.66	0/1256
All	All	0.44	0/5296	0.70	1/7170 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	337	LEU	CA-CB-CG	5.38	127.68	115.30

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	800	0	785	68	0
1	C	800	0	785	74	0
1	E	800	0	785	66	0
2	B	932	0	904	101	0
2	D	942	0	926	73	0
2	F	911	0	885	60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5185	0	5070	401	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 39.

The worst 5 of 401 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:306:VAL:HG11	1:C:311:ILE:HG12	1.41	1.02
1:E:347:LEU:H	1:E:347:LEU:HD12	1.30	0.96
2:B:317:LYS:HG3	2:B:318:ASP:H	1.31	0.94
1:C:293:CYS:HA	1:C:375:TYR:HD2	1.31	0.94
1:C:283:ILE:HG12	1:C:359:LEU:CD1	2.00	0.92

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	
1	A	99/101 (98%)	79 (80%)	11 (11%)	9 (9%)	1	3
1	C	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	2	13
1	E	99/101 (98%)	81 (82%)	15 (15%)	3 (3%)	4	24
2	B	113/115 (98%)	82 (73%)	22 (20%)	9 (8%)	1	5
2	D	113/115 (98%)	92 (81%)	11 (10%)	10 (9%)	1	3
2	F	110/115 (96%)	91 (83%)	12 (11%)	7 (6%)	1	9
All	All	633/648 (98%)	509 (80%)	81 (13%)	43 (7%)	1	7

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	SER
1	A	377	PRO
2	B	275	LYS
2	B	288	ASN
2	B	305	ARG

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	
1	A	92/92 (100%)	86 (94%)	6 (6%)	17	48
1	C	92/92 (100%)	83 (90%)	9 (10%)	8	28
1	E	92/92 (100%)	86 (94%)	6 (6%)	17	48
2	B	102/104 (98%)	89 (87%)	13 (13%)	4	19
2	D	104/104 (100%)	88 (85%)	16 (15%)	2	12
2	F	100/104 (96%)	91 (91%)	9 (9%)	9	32
All	All	582/588 (99%)	523 (90%)	59 (10%)	7	27

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	348	GLU
2	D	301	THR
2	F	319	VAL
1	C	374	THR
2	D	250	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	306	GLN
2	B	320	ASN
1	E	307	GLN
2	B	274	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	306	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 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 (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, 95th 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(Å²)	Q<0.9
1	A	101/101 (100%)	0.05	2 (1%)	65	50	66, 102, 124, 140	0
1	C	101/101 (100%)	-0.24	1 (0%)	82	73	56, 83, 111, 131	0
1	E	101/101 (100%)	-0.07	1 (0%)	82	73	79, 115, 138, 140	0
2	B	115/115 (100%)	-0.19	0	100	100	49, 70, 115, 136	0
2	D	115/115 (100%)	-0.22	0	100	100	51, 71, 116, 140	0
2	F	112/115 (97%)	-0.22	1 (0%)	84	75	57, 88, 115, 135	0
All	All	645/648 (99%)	-0.15	5 (0%)	86	78	49, 87, 131, 140	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	278	THR	2.6
1	C	278	THR	2.5
1	A	278	THR	2.3
2	F	245	ALA	2.1
1	A	279	SER	2.0

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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.