



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 08:09 PM UTC

PDB ID : 4E3C / pdb\_00004e3c  
Title : X-ray crystal structure of human IKK2 in an active conformation  
Authors : Polley, S.; Huang, D.B.; Hauenstein, A.V.; Ghosh, G.; Huxford, T.  
Deposited on : 2012-03-09  
Resolution : 3.98 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:

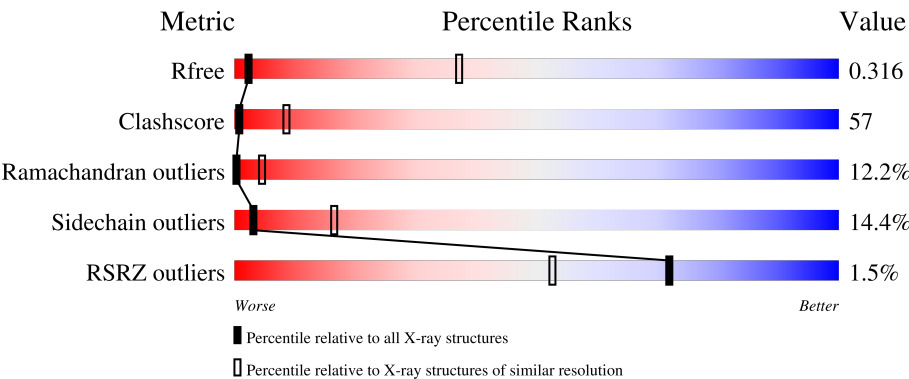
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.98 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))
$R_{free}$	180053	1016 (4.18-3.78)
Clashscore	190562	1007 (4.16-3.80)
Ramachandran outliers	187476	1000 (4.18-3.78)
Sidechain outliers	187428	1131 (4.20-3.76)
RSRZ outliers	180081	1016 (4.18-3.78)

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	669	<div><div>2%</div><div><div></div><div>26%</div><div>49%</div><div>16%</div><div>7%</div></div></div>
1	B	669	<div><div>%</div><div><div></div><div>26%</div><div>48%</div><div>18%</div><div>6%</div></div></div>
1	C	669	<div><div>2%</div><div><div></div><div>26%</div><div>49%</div><div>17%</div><div>7%</div></div></div>
1	D	669	<div><div>%</div><div><div></div><div>25%</div><div>51%</div><div>15%</div><div>7%</div></div></div>
1	E	669	<div><div>%</div><div><div></div><div>25%</div><div>51%</div><div>15%</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	669	<div><div><div>%</div><div><div></div><div>26%</div><div>50%</div><div>16%</div><div>• 7%</div></div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30416 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 Inhibitor of nuclear factor kappa-B kinase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	B	632	Total	C	N	O	S	0	0	0
			5116	3219	904	959	34			
1	C	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	D	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	E	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	F	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASN	-	expression tag	UNP O14920
A	2	LEU	-	expression tag	UNP O14920
A	3	TYR	-	expression tag	UNP O14920
A	4	PHE	-	expression tag	UNP O14920
A	5	GLN	-	expression tag	UNP O14920
A	6	GLY	-	expression tag	UNP O14920
A	7	ALA	-	expression tag	UNP O14920
A	8	MET	-	expression tag	UNP O14920
A	9	GLY	-	expression tag	UNP O14920
A	10	SER	-	expression tag	UNP O14920
A	177	GLU	SER	engineered mutation	UNP O14920
A	181	GLU	SER	engineered mutation	UNP O14920
B	1	ASN	-	expression tag	UNP O14920
B	2	LEU	-	expression tag	UNP O14920
B	3	TYR	-	expression tag	UNP O14920
B	4	PHE	-	expression tag	UNP O14920
B	5	GLN	-	expression tag	UNP O14920

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	GLY	-	expression tag	UNP O14920
B	7	ALA	-	expression tag	UNP O14920
B	8	MET	-	expression tag	UNP O14920
B	9	GLY	-	expression tag	UNP O14920
B	10	SER	-	expression tag	UNP O14920
B	177	GLU	SER	engineered mutation	UNP O14920
B	181	GLU	SER	engineered mutation	UNP O14920
C	1	ASN	-	expression tag	UNP O14920
C	2	LEU	-	expression tag	UNP O14920
C	3	TYR	-	expression tag	UNP O14920
C	4	PHE	-	expression tag	UNP O14920
C	5	GLN	-	expression tag	UNP O14920
C	6	GLY	-	expression tag	UNP O14920
C	7	ALA	-	expression tag	UNP O14920
C	8	MET	-	expression tag	UNP O14920
C	9	GLY	-	expression tag	UNP O14920
C	10	SER	-	expression tag	UNP O14920
C	177	GLU	SER	engineered mutation	UNP O14920
C	181	GLU	SER	engineered mutation	UNP O14920
D	1	ASN	-	expression tag	UNP O14920
D	2	LEU	-	expression tag	UNP O14920
D	3	TYR	-	expression tag	UNP O14920
D	4	PHE	-	expression tag	UNP O14920
D	5	GLN	-	expression tag	UNP O14920
D	6	GLY	-	expression tag	UNP O14920
D	7	ALA	-	expression tag	UNP O14920
D	8	MET	-	expression tag	UNP O14920
D	9	GLY	-	expression tag	UNP O14920
D	10	SER	-	expression tag	UNP O14920
D	177	GLU	SER	engineered mutation	UNP O14920
D	181	GLU	SER	engineered mutation	UNP O14920
E	1	ASN	-	expression tag	UNP O14920
E	2	LEU	-	expression tag	UNP O14920
E	3	TYR	-	expression tag	UNP O14920
E	4	PHE	-	expression tag	UNP O14920
E	5	GLN	-	expression tag	UNP O14920
E	6	GLY	-	expression tag	UNP O14920
E	7	ALA	-	expression tag	UNP O14920
E	8	MET	-	expression tag	UNP O14920
E	9	GLY	-	expression tag	UNP O14920
E	10	SER	-	expression tag	UNP O14920
E	177	GLU	SER	engineered mutation	UNP O14920

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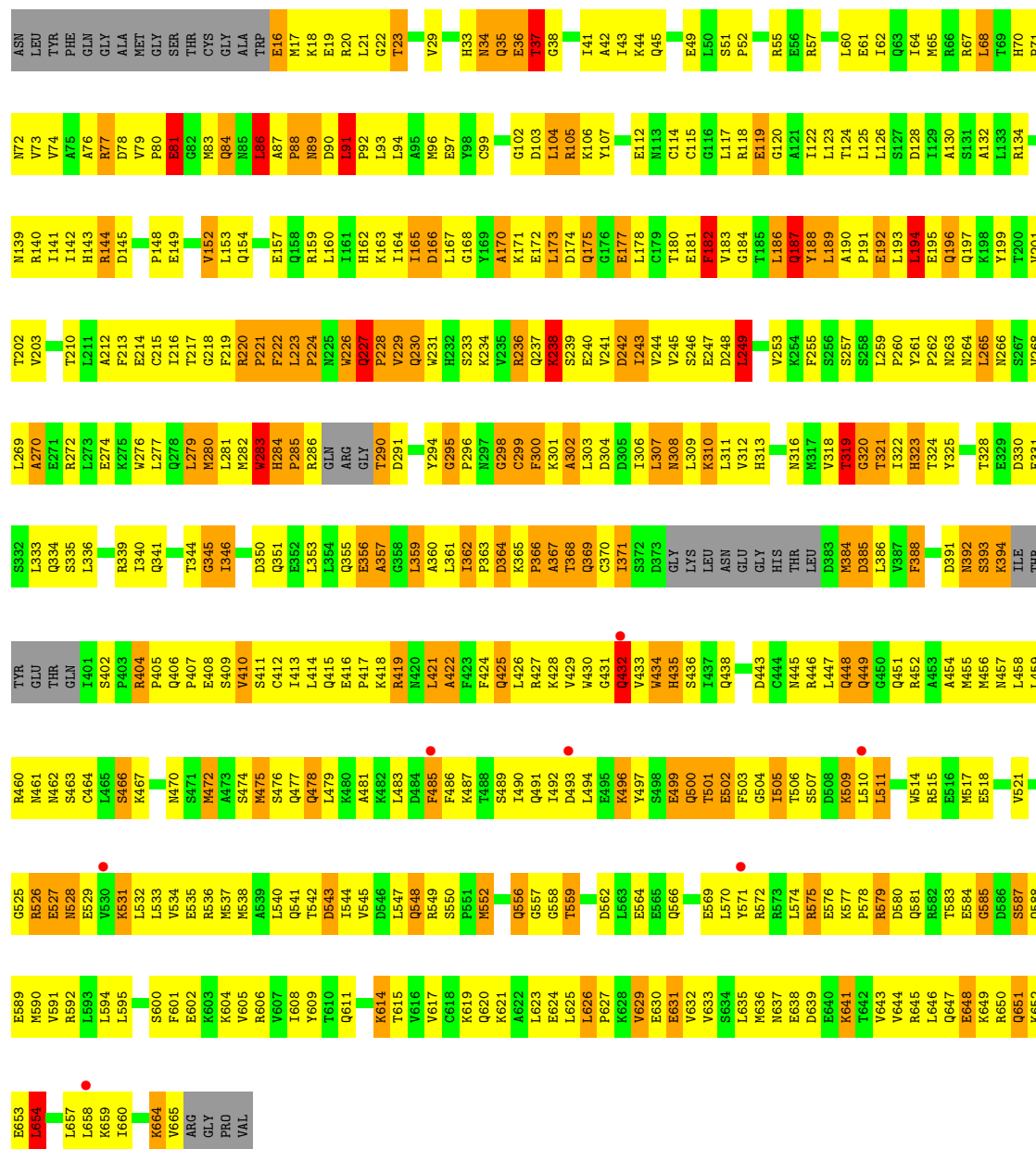
Chain	Residue	Modelled	Actual	Comment	Reference
E	181	GLU	SER	engineered mutation	UNP O14920
F	1	ASN	-	expression tag	UNP O14920
F	2	LEU	-	expression tag	UNP O14920
F	3	TYR	-	expression tag	UNP O14920
F	4	PHE	-	expression tag	UNP O14920
F	5	GLN	-	expression tag	UNP O14920
F	6	GLY	-	expression tag	UNP O14920
F	7	ALA	-	expression tag	UNP O14920
F	8	MET	-	expression tag	UNP O14920
F	9	GLY	-	expression tag	UNP O14920
F	10	SER	-	expression tag	UNP O14920
F	177	GLU	SER	engineered mutation	UNP O14920
F	181	GLU	SER	engineered mutation	UNP O14920



K659  
I660  
A661  
C662  
S663  
K664  
V665  
ARG  
GLY  
PRO  
VAL

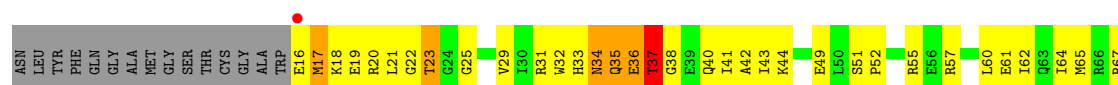
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

Chain B:  26% 48% 18% 6%



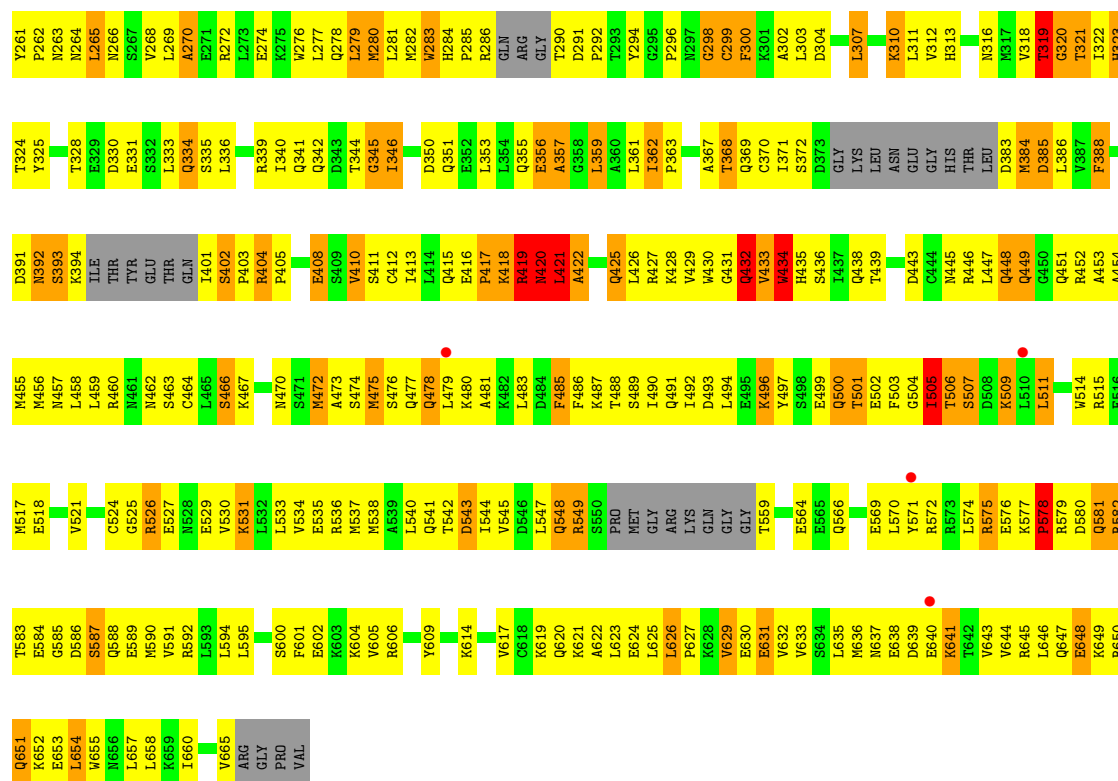
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

Chain C:  26% 49% 17% 7%

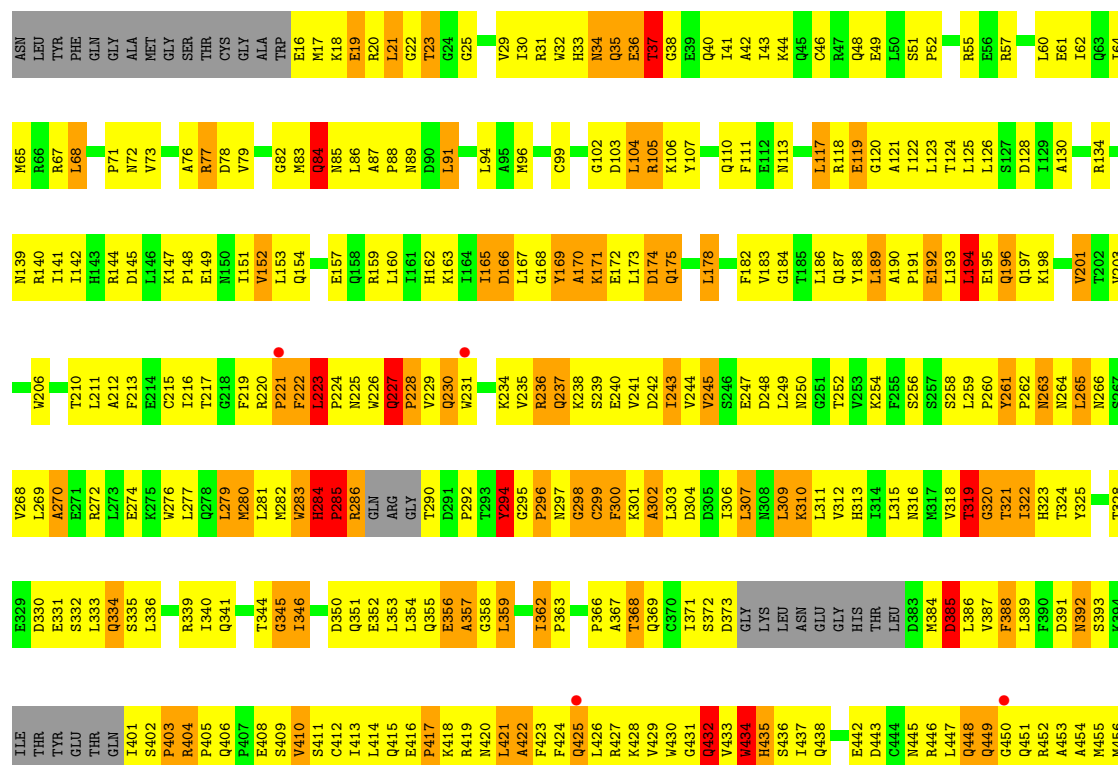


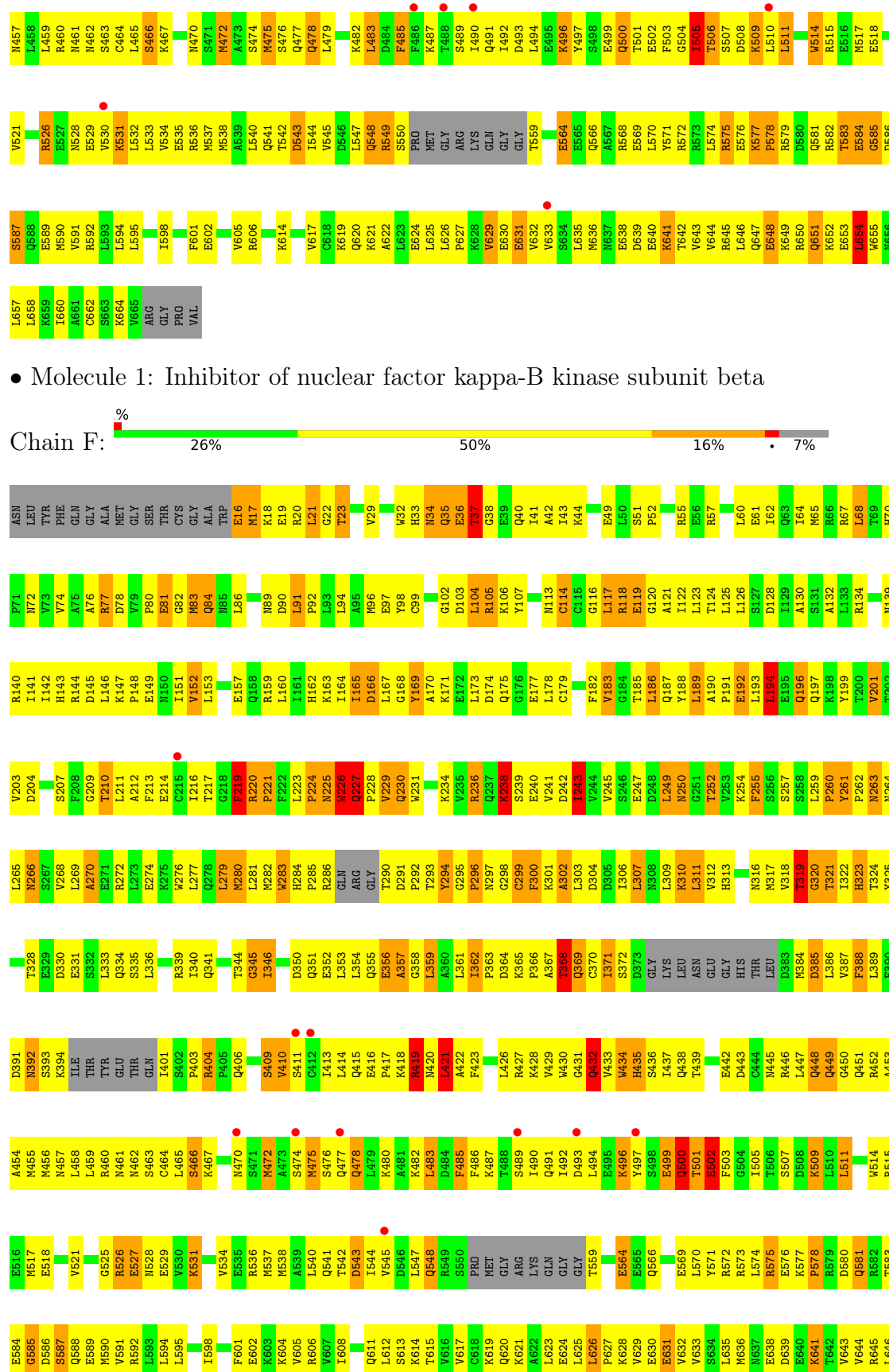






● Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta





Q647	E648	R649	Q650	Q651	K652	E653	L654	L657	L658	K659	I660	A661	S662	S663	K664	V665	ARG	GLY	PRO	VAL
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.81Å 170.81Å 509.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.98 29.84 – 3.98	Depositor EDS
% Data completeness (in resolution range)	81.0 (29.84-3.98) 88.4 (29.84-3.98)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 4.00Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.267 , 0.299 0.285 , 0.316	Depositor DCC
$R_{free}$ test set	2388 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	113.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 156.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	30416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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](#)

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	0.62	0/5142	0.94	20/6937 (0.3%)
1	B	0.60	0/5200	0.91	18/7014 (0.3%)
1	C	0.57	1/5142 (0.0%)	0.88	8/6937 (0.1%)
1	D	0.57	0/5142	0.91	10/6937 (0.1%)
1	E	0.55	0/5142	0.88	10/6937 (0.1%)
1	F	0.51	0/5142	0.87	6/6937 (0.1%)
All	All	0.57	1/30910 (0.0%)	0.90	72/41699 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	387	VAL	CA-CB	5.28	1.61	1.53

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ARG	NE-CZ-NH2	13.31	131.18	119.20
1	B	144	ARG	NE-CZ-NH2	12.29	130.26	119.20
1	A	283	TRP	N-CA-C	12.12	118.72	108.78
1	D	118	ARG	NE-CZ-NH1	-12.12	109.38	121.50
1	B	144	ARG	NE-CZ-NH1	-11.66	109.84	121.50

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	5060	0	5109	624	0
1	B	5116	0	5169	611	0
1	C	5060	0	5109	563	0
1	D	5060	0	5109	603	0
1	E	5060	0	5107	597	0
1	F	5060	0	5107	626	0
All	All	30416	0	30710	3492	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 3492 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:B:419:ARG:NH1	1:B:419:ARG:HB2	1.55	1.18
1:B:366:PRO:HB2	1:B:368:THR:HG23	1.29	1.14
1:C:496:LYS:HE2	1:C:654:LEU:HD21	1.20	1.14
1:F:626:LEU:H	1:F:627:PRO:HD2	1.13	1.13
1:D:479:LEU:HD11	1:D:641:LYS:HG2	1.28	1.11

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	
1	A	614/669 (92%)	427 (70%)	112 (18%)	75 (12%)	0	4
1	B	624/669 (93%)	411 (66%)	133 (21%)	80 (13%)	0	4
1	C	614/669 (92%)	423 (69%)	117 (19%)	74 (12%)	0	4
1	D	614/669 (92%)	421 (69%)	119 (19%)	74 (12%)	0	4
1	E	614/669 (92%)	417 (68%)	121 (20%)	76 (12%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	614/669 (92%)	421 (69%)	120 (20%)	73 (12%)	0	5
All	All	3694/4014 (92%)	2520 (68%)	722 (20%)	452 (12%)	0	4

5 of 452 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	MET
1	A	35	GLN
1	A	92	PRO
1	A	166	ASP
1	A	182	PHE

### 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	567/601 (94%)	483 (85%)	84 (15%)	3	16
1	B	572/601 (95%)	488 (85%)	84 (15%)	3	16
1	C	567/601 (94%)	488 (86%)	79 (14%)	3	17
1	D	567/601 (94%)	487 (86%)	80 (14%)	3	17
1	E	567/601 (94%)	488 (86%)	79 (14%)	3	17
1	F	567/601 (94%)	481 (85%)	86 (15%)	3	15
All	All	3407/3606 (94%)	2915 (86%)	492 (14%)	3	16

5 of 492 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	528	ASN
1	F	304	ASP
1	D	368	THR
1	F	261	TYR
1	F	507	SER



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	278	GLN
1	F	72	ASN
1	D	70	HIS
1	F	70	HIS
1	F	369	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 [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	624/669 (93%)	0.08	14 (2%) 62 45	56, 129, 201, 287	0
1	B	632/669 (94%)	0.01	7 (1%) 78 59	56, 130, 204, 256	0
1	C	624/669 (93%)	-0.04	11 (1%) 67 49	64, 133, 201, 267	0
1	D	624/669 (93%)	-0.11	5 (0%) 82 65	62, 132, 201, 286	0
1	E	624/669 (93%)	-0.00	10 (1%) 70 51	63, 134, 205, 264	0
1	F	624/669 (93%)	0.06	10 (1%) 70 51	64, 144, 206, 256	0
All	All	3752/4014 (93%)	-0.00	57 (1%) 72 52	56, 133, 204, 287	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	493	ASP	3.8
1	D	571	TYR	3.7
1	C	510	LEU	3.6
1	F	497	TYR	3.6
1	B	571	TYR	3.5

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.