



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:38 PM GMT

PDB ID : 1GJI  
Title : Crystal structure of c-Rel bound to DNA  
Authors : Huang, D.B.; Chen, Y.Q.; Ruetsche, M.; Phelps, C.B.; Ghosh, G.  
Deposited on : 2001-05-30  
Resolution : 2.85 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

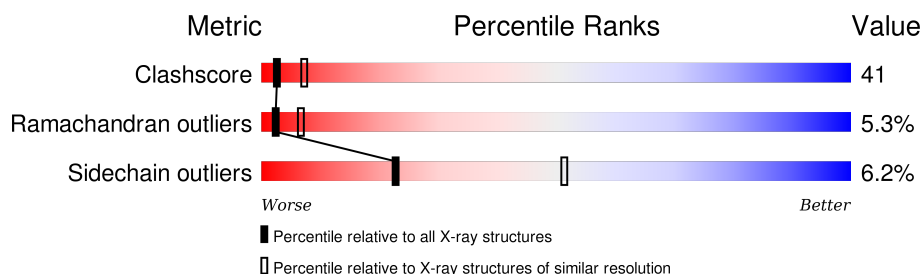
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	20	
2	D	20	
3	A	275	
3	B	275	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6114 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 IL-2 CD28RE DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	20	Total	C	N	O	P	0	20	0
			826	396	162	230	38			

- Molecule 2 is a DNA chain called IL-2 CD28RE DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	20	Total	C	N	O	P	0	20	0
			802	390	132	242	38			

- Molecule 3 is a protein called C-REL PROTO-ONCOGENE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	275	Total	C	N	O	S	0	0	0
			2243	1420	398	415	10			
3	B	275	Total	C	N	O	S	0	0	0
			2243	1420	398	415	10			

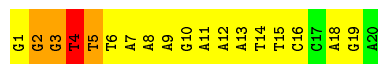
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

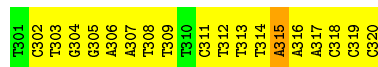
#### • Molecule 1: IL-2 CD28RE DNA

Chain C: 



#### • Molecule 2: IL-2 CD28RE DNA

Chain D: 



H159	G160	M161	Y162	P167	P168	L169	I170	S171	M172	P173	I174	Y175	D176	M177	R178	A179	T182	A183	E184	L185	R186	R189	V190	M191	K192	V197	K198	G199	G200	I205	L206	G207	D208	K212	D213	D214	I215	R218	L221	D222	M223	M224	G228	S229	F230	D234	V235	H236	R237
A240	I241	V242	F243	P247	F248	L249	R250	D251	I252	T253	E254	P255	I256	T257	Q261	L262	R263	R264	D267	Q268	E269	V270	S271	E272	P273	R277	D281																						

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.32Å 99.32Å 196.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.85	Depositor
% Data completeness (in resolution range)	79.2 (25.00-2.85)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.227 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

## 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	C	0.82	2/930 (0.2%)	1.00	4/1434 (0.3%)
2	D	0.60	0/894	0.91	0/1374
3	A	0.45	0/2296	0.70	0/3104
3	B	0.41	0/2296	0.69	2/3104 (0.1%)
All	All	0.53	2/6416 (0.0%)	0.78	6/9016 (0.1%)

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	2
2	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2[A]	DG	C2-N2	-5.65	1.28	1.34
1	C	2[B]	DG	C2-N2	-5.65	1.28	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4[A]	DT	N1-C1'-C2'	5.29	122.64	112.60
1	C	4[B]	DT	N1-C1'-C2'	5.29	122.64	112.60
1	C	5[A]	DT	C3'-C2'-C1'	-5.26	96.19	102.50
1	C	5[B]	DT	C3'-C2'-C1'	-5.26	96.19	102.50
3	B	228	GLY	N-CA-C	-5.09	100.37	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	3[A]	DG	Sidechain
1	C	4[A]	DT	Sidechain
2	D	315[A]	DA	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	826	0	432	71	0
2	D	802	0	433	86	0
3	A	2243	0	2223	171	0
3	B	2243	0	2223	179	0
All	All	6114	0	5311	471	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 41.

The worst 5 of 471 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:319[A]:DC:H2''	2:D:320[A]:DC:C5'	1.55	1.33
2:D:302[B]:DC:H2''	2:D:303[B]:DT:H5''	1.20	1.19
1:C:3[A]:DG:N2	2:D:319[A]:DC:O2	1.84	1.11
2:D:319[A]:DC:C2'	2:D:320[A]:DC:H5''	1.81	1.10
1:C:5[A]:DT:H2''	1:C:6[A]:DT:O5'	1.45	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	273/275 (99%)	223 (82%)	34 (12%)	16 (6%)	2	5
3	B	273/275 (99%)	220 (81%)	40 (15%)	13 (5%)	3	9
All	All	546/550 (99%)	443 (81%)	74 (14%)	29 (5%)	2	7

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	95	GLU
3	A	141	GLU
3	A	158	GLU
3	B	95	GLU
3	B	133	GLU

### 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	252/252 (100%)	236 (94%)	16 (6%)	22	50
3	B	252/252 (100%)	237 (94%)	15 (6%)	24	53
All	All	504/504 (100%)	473 (94%)	31 (6%)	23	51

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	257	THR
3	B	9	ILE
3	B	249	LEU
3	A	270	VAL
3	B	20	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	43	ASN
3	B	68	ASN
3	B	232	GLN
3	B	50	GLN
3	A	103	ASN

### 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.