

# wwPDB X-ray Structure Validation Summary Report (i)

#### Jun 13, 2024 – 10:16 AM EDT

PDB ID : 4JBK

Title: Molecular basis for abrogation of activation of pro-inflammatory cytokines Authors: Ru, H.; Ni, X.; Crowley, C.; Zhao, L.; Ding, W.; Hung, L.-W.; Shaw, N.;

Cheng, G.; Liu, Z.-J.

Deposited on : 2013-02-19

Resolution : 2.96 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*A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.20.1 \end{array}$ 

EDS : 2.36.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

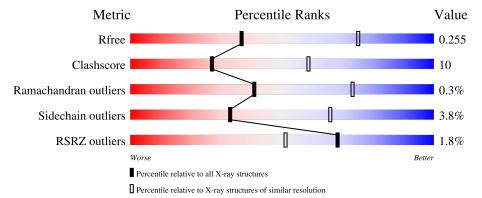
Validation Pipeline (wwPDB-VP) : 2.36.2

## 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 2.96 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 >=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	198	73%	21%	
1	В	198	69%	25%	
1	С	198	71%	22%	• 5%
1	D	198	69%	25%	• 6%
2	Е	14	43% 50%		7%

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Mol	Chain	Length	Quality of chain			
2	F	14	43%	57%		
2	G	14	64%	14%	21%	
2	Н	14	57%	36%	7%	



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7235 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 Interferon-activable protein 202.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	192	Total	С	N	О	S	0	0	0
1	A	192	1546	992	262	287	5	0	0	U
1	В	190	Total	С	N	О	S	0	0	0
1	Ъ	190	1524	979	256	284	5	0	0	U
1	С	188	Total	С	N	О	S	0	0	0
1		100	1511	971	253	282	5	0	U	U
1	D	187	Total	С	N	О	S	0	0	0
1	ע	107	1506	966	253	282	5	U	U	U

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	expression tag	UNP Q9R002
A	98	MET	ILE	SEE REMARK 999	UNP Q9R002
A	99	PHE	ILE	SEE REMARK 999	UNP Q9R002
A	161	GLU	LYS	SEE REMARK 999	UNP Q9R002
В	2	MET	-	expression tag	UNP Q9R002
В	98	MET	ILE	SEE REMARK 999	UNP Q9R002
В	99	PHE	ILE	SEE REMARK 999	UNP Q9R002
В	161	GLU	LYS	SEE REMARK 999	UNP Q9R002
С	2	MET	-	expression tag	UNP Q9R002
С	98	MET	ILE	SEE REMARK 999	UNP Q9R002
С	99	PHE	ILE	SEE REMARK 999	UNP Q9R002
С	161	GLU	LYS	SEE REMARK 999	UNP Q9R002
D	2	MET	-	expression tag	UNP Q9R002
D	98	MET	ILE	SEE REMARK 999	UNP Q9R002
D	99	PHE	ILE	SEE REMARK 999	UNP Q9R002
D	161	GLU	LYS	SEE REMARK 999	UNP Q9R002

• Molecule 2 is a DNA chain called DNA (5'-D(P\*GP\*GP\*AP\*AP\*TP\*TP\*AP\*AP\*AP\*TP\*TP\*AP\*AP\*TP\*TP\*CP\*C)-3').



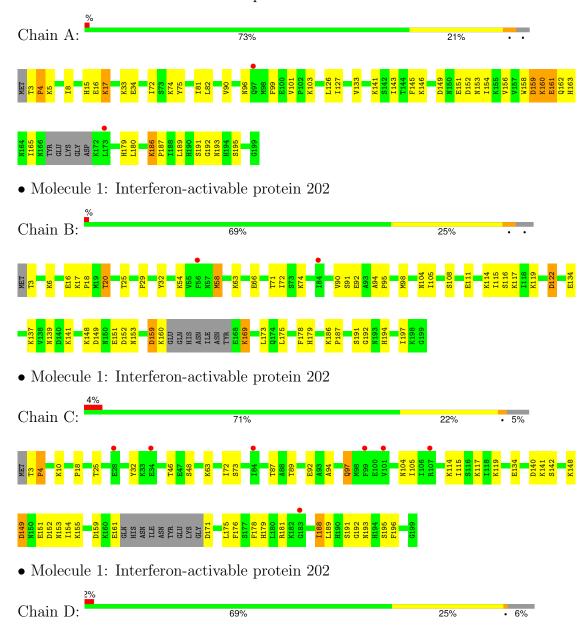
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Е	14	Total	С	N	О	Р	0	0	0
	12	14	287	138	51	84	14	0	0	
9	F	14	Total	С	N	О	Р	0	0	0
2	I.	14	287	138	51	84	14			
2	G	14	Total	С	N	О	Р	0	0	0
2	G	14	287	138	51	84	14	U	0	U
9	Н	14	Total	С	N	О	Р	0	0	0
	11	14	287	138	51	84	14	U	0	U



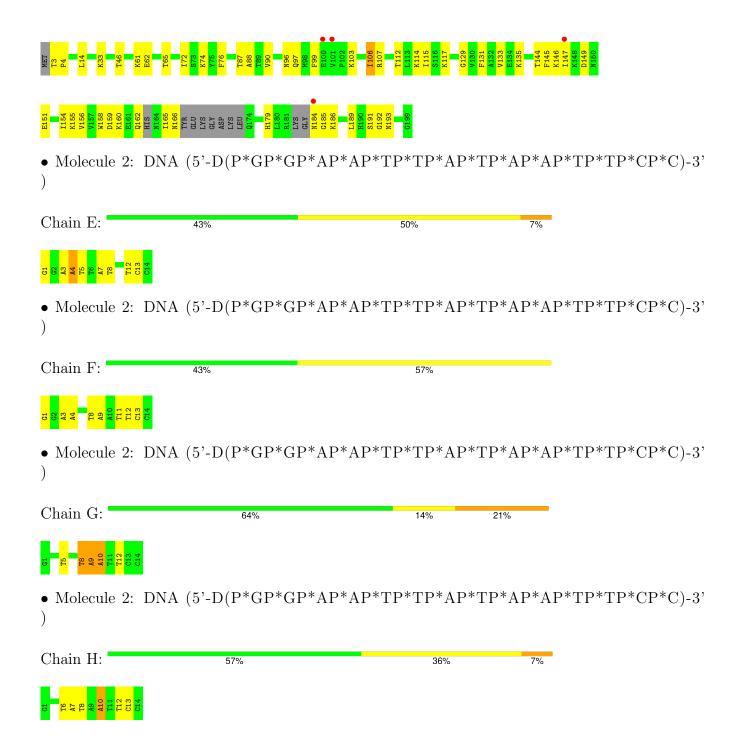
## 3 Residue-property plots (i)

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: Interferon-activable protein 202









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	106.30Å 109.94Å 106.14Å	D t
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $120.03^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	47.17 - 2.96	Depositor
Resolution (A)	47.17  -  2.96	EDS
% Data completeness	99.0 (47.17-2.96)	Depositor
(in resolution range)	96.5 (47.17-2.96)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sum}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	5.10 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
Ρ. Р.	0.220 , 0.253	Depositor
$R, R_{free}$	0.223 , $0.255$	DCC
$R_{free}$ test set	1998 reflections (9.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.29 , 40.8	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.49, < L^2> = 0.31$	Xtriage
	0.018  for  k,h,-1/2*h-1/2*k-l	
Estimated twinning fraction	0.008  for -k,-h,-1/2*h+1/2*k-l	Xtriage
	0.016  for h,-k,-h-l	
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7235	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.66% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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	Bo	nd lengths	В	ond angles
WIOI			# Z  > 5	RMSZ	# Z >5
1	A	0.35	0/1575	0.53	0/2112
1	В	0.44	0/1552	0.59	1/2079~(0.0%)
1	С	0.32	0/1539	0.53	0/2063
1	D	0.30	0/1532	0.51	0/2053
2	Е	0.51	0/321	1.51	4/493 (0.8%)
2	F	0.56	0/321	1.32	1/493 (0.2%)
2	G	1.13	4/321 (1.2%)	2.17	21/493 (4.3%)
2	Н	0.57	0/321	1.32	3/493 (0.6%)
All	All	0.45	4/7482 (0.1%)	0.86	30/10279 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}( ext{\AA})$
2	G	9	DA	C3'-O3'	7.91	1.54	1.44
2	G	10	DA	C5'-C4'	6.10	1.58	1.51
2	G	8	DT	C3'-O3'	-5.74	1.36	1.44
2	G	10	DA	C3'-O3'	-5.46	1.36	1.44

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
2	G	10	DA	P-O5'-C5'	12.63	141.11	120.90
2	G	10	DA	O5'-C5'-C4'	12.35	141.88	111.00
2	G	10	DA	O5'-P-OP2	11.02	123.92	110.70
2	G	9	DA	C4'-C3'-C2'	-10.87	93.32	103.10
2	Е	4	DA	OP1-P-O3'	-10.71	81.65	105.20

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	1546	0	1583	32	0
1	В	1524	0	1565	39	0
1	С	1511	0	1549	33	0
1	D	1506	0	1534	32	0
2	Е	287	0	160	5	0
2	F	287	0	160	5	0
2	G	287	0	160	4	0
2	Н	287	0	160	4	0
All	All	7235	0	6871	144	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 10.

The worst 5 of 144 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:D:114:LYS:H	1:D:117:LYS:HE3	1.32	0.94
1:C:114:LYS:HZ1	1:C:151:GLU:H	1.16	0.94
1:B:173:LEU:HD11	1:B:197:ILE:HG23	1.53	0.88
1:A:160:LYS:CA	1:A:160:LYS:HE2	2.01	0.87
1:D:33:LYS:NZ	1:D:193:ASN:OD1	2.08	0.86

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	Percen	ntiles
1	A	188/198 (95%)	184 (98%)	3 (2%)	1 (0%)	29	64
1	В	186/198 (94%)	183 (98%)	3 (2%)	0	100	100
1	C	184/198 (93%)	178 (97%)	5 (3%)	1 (0%)	29	64
1	D	179/198 (90%)	172 (96%)	7 (4%)	0	100	100
All	All	737/792~(93%)	717 (97%)	18 (2%)	2 (0%)	41	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	4	PRO
1	A	4	PRO

#### 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	Percei	ntiles
1	A	174/179 (97%)	167 (96%)	7 (4%)	31	64
1	В	171/179 (96%)	163 (95%)	8 (5%)	26	59
1	С	170/179 (95%)	163 (96%)	7 (4%)	30	64
1	D	170/179 (95%)	166 (98%)	4 (2%)	49	77
All	All	685/716 (96%)	659 (96%)	26 (4%)	33	66

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	169	LYS
1	С	97	GLN
1	D	133	VAL
1	С	87	THR
1	С	140	ASP

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



Mol	Chain	Res	Type
1	С	77	ASN
1	С	139	ASN
1	D	179	HIS
1	D	166	ASN
1	A	193	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 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,  $95^{th}$  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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	192/198~(96%)	0.03	2 (1%) 82 68	50, 76, 111, 124	0
1	В	190/198 (95%)	0.01	2 (1%) 80 65	49, 77, 109, 120	0
1	С	188/198 (94%)	0.07	7 (3%) 41 27	52, 76, 110, 137	0
1	D	187/198 (94%)	0.17	4 (2%) 63 46	49, 77, 111, 122	0
2	Е	14/14 (100%)	-0.10	0 100 100	55, 68, 74, 90	0
2	F	14/14 (100%)	-0.02	0 100 100	53, 68, 74, 92	0
2	G	14/14 (100%)	0.08	0 100 100	54, 67, 74, 90	0
2	Н	14/14 (100%)	-0.28	0 100 100	58, 71, 77, 93	0
All	All	813/848 (95%)	0.06	15 (1%) 68 51	49, 75, 111, 137	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	183	GLY	4.2
1	С	28	GLU	2.8
1	A	97	GLN	2.8
1	С	34	GLU	2.7
1	В	84	ILE	2.6

### 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.

