



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:36 pm BST

PDB ID : 1INR  
Title : CYTOKINE SYNTHESIS  
Authors : Walter, M.R.  
Deposited on : 1995-07-31  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

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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  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

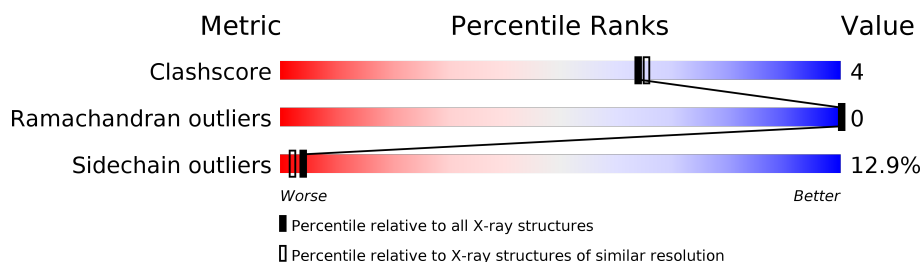
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	160	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1114 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 INTERLEUKIN-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	132	1072	688	181	195	8	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total	O	0	0
			42	42		



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.37Å 36.37Å 220.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	83.0 (10.00-2.00)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.221 , 0.337	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

## 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	1.09	1/1087 (0.1%)	2.06	29/1453 (2.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	ARG	CZ-NH1	5.02	1.39	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ARG	NE-CZ-NH2	-17.20	111.70	120.30
1	A	102	ARG	NE-CZ-NH2	-17.14	111.73	120.30
1	A	102	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	A	24	ARG	NE-CZ-NH2	-11.58	114.51	120.30
1	A	137	TYR	CB-CG-CD1	-10.59	114.65	121.00
1	A	27	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	A	91	VAL	CG1-CB-CG2	-9.18	96.21	110.90
1	A	81	GLU	CA-CB-CG	9.04	133.29	113.40
1	A	102	ARG	CA-CB-CG	-7.73	96.39	113.40
1	A	54	GLU	CA-CB-CG	-7.71	96.43	113.40
1	A	154	MET	CA-CB-CG	7.33	125.76	113.30
1	A	32	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	A	46	LEU	CA-CB-CG	7.21	131.88	115.30
1	A	34	LYS	CA-CB-CG	7.01	128.81	113.40
1	A	145	ILE	CG1-CB-CG2	-6.69	96.68	111.40
1	A	144	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	81	GLU	N-CA-CB	-6.16	99.52	110.60
1	A	87	ILE	CA-CB-CG1	-5.94	99.71	111.00
1	A	19	LEU	CB-CG-CD1	-5.94	100.90	111.00
1	A	106	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	A	153	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	A	106	ARG	N-CA-CB	-5.62	100.49	110.60
1	A	112	LEU	CB-CG-CD1	-5.61	101.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	MET	CG-SD-CE	5.23	108.57	100.20
1	A	100	THR	CA-CB-CG2	5.20	119.68	112.40
1	A	19	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	46	LEU	CB-CA-C	5.14	119.96	110.20
1	A	55	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	106	ARG	CB-CG-CD	-5.01	98.58	111.60

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	1072	0	1081	9	0
2	A	42	0	0	0	0
All	All	1114	0	1081	9	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 4.

All (9) 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:A:65:LEU:HD23	1:A:112:LEU:HD21	1.74	0.69
1:A:100:THR:HG22	1:A:104:ARG:HH11	1.73	0.53
1:A:149:TYR:O	1:A:152:ALA:HB3	2.12	0.50
1:A:117:LYS:NZ	1:A:122:GLU:HB2	2.32	0.45
1:A:55:ASP:O	1:A:61:GLY:HA2	2.18	0.43
1:A:150:ILE:O	1:A:154:MET:HG2	2.18	0.43
1:A:106:ARG:HH11	1:A:106:ARG:HD2	1.67	0.43
1:A:60:LEU:HA	1:A:63:GLN:HE21	1.85	0.42
1:A:84:ASP:HA	1:A:85:PRO:HD2	1.79	0.42

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	126/160 (79%)	123 (98%)	3 (2%)	0	100 100

There are no Ramachandran outliers to report.

### 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	116/145 (80%)	101 (87%)	15 (13%)	4 2

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	81	GLU
1	A	98	LEU
1	A	102	ARG
1	A	103	LEU
1	A	105	LEU
1	A	117	LYS
1	A	119	LYS
1	A	130	LYS
1	A	133	GLU
1	A	145	ILE
1	A	154	MET
1	A	155	THR

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Mol	Chain	Res	Type
1	A	158	ILE
1	A	159	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	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](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.