



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:08 PM GMT

PDB ID : 1NLW  
Title : Crystal structure of Mad-Max recognizing DNA  
Authors : Nair, S.K.; Burley, S.K.  
Deposited on : 2003-01-07  
Resolution : 2.00 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

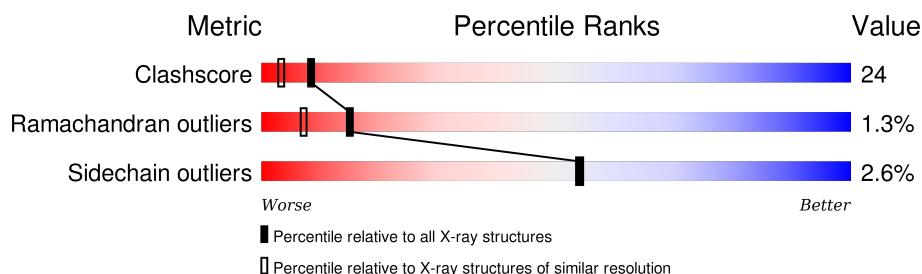
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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. 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	F	18	<div> <div>17%</div> <div>83%</div> </div>
1	G	18	<div> <div>44%</div> <div>56%</div> </div>
1	H	18	<div> <div>50%</div> <div>50%</div> </div>
1	J	18	<div> <div>61%</div> <div>39%</div> </div>
2	A	80	<div> <div>65%</div> <div>30%</div> <div>• •</div> </div>
2	D	80	<div> <div>58%</div> <div>36%</div> <div>• •</div> </div>
3	B	76	<div> <div>61%</div> <div>36%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	76	 A horizontal bar chart showing the quality of chain E. The bar is divided into two segments: a green segment on the left representing 61% and a yellow segment on the right representing 37%. A small grey segment is visible at the far right end of the bar. The percentage values '61%' and '37%' are printed below the green and yellow segments respectively. A small black dot is located at the end of the grey segment.

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4212 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 5'-D(\*GP\*AP\*GP\*TP\*AP\*GP\*CP\*AP\*CP\*GP\*TP\*GP\*CP\*TP\*AP\*CP\*TP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	18	Total	C	N	O	P	0	0	0
			366	175	68	106	17			
1	G	18	Total	C	N	O	P	0	0	0
			366	175	68	106	17			
1	H	18	Total	C	N	O	P	0	0	0
			366	175	68	106	17			
1	J	18	Total	C	N	O	P	0	0	0
			366	175	68	106	17			

- Molecule 2 is a protein called MAD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	79	Total	C	N	O	S	0	0	0
			634	388	133	112	1			
2	D	77	Total	C	N	O	S	0	0	0
			609	376	122	110	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	CYS	ENGINEERED	UNP Q05195
A	33	ASP	GLU	VARIANT	UNP Q05195
A	56	SER	CYS	ENGINEERED	UNP Q05195
D	520	SER	CYS	ENGINEERED	UNP Q05195
D	533	ASP	GLU	VARIANT	UNP Q05195
D	556	SER	CYS	ENGINEERED	UNP Q05195

- Molecule 3 is a protein called MAX PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	76	Total 637	C 387	N 131	O 118	S 1	0	0	0
3	E	74	Total 617	C 375	N 125	O 116	S 1	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total 36	O 36	0	0
4	B	38	Total 38	O 38	0	0
4	D	41	Total 41	O 41	0	0
4	E	28	Total 28	O 28	0	0
4	F	26	Total 26	O 26	0	0
4	G	38	Total 38	O 38	0	0
4	H	23	Total 23	O 23	0	0
4	J	21	Total 21	O 21	0	0

### 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: 5'-D(\*GP\*AP\*GP\*TP\*AP\*GP\*CP\*AP\*CP\*GP\*TP\*GP\*CP\*TP\*AP\*CP\*TP\*C)-3'

Chain F: 



- Molecule 1: 5'-D(\*GP\*AP\*GP\*TP\*AP\*GP\*CP\*AP\*CP\*GP\*TP\*GP\*CP\*TP\*AP\*CP\*TP\*C)-3'

Chain G: 



- Molecule 1: 5'-D(\*GP\*AP\*GP\*TP\*AP\*GP\*CP\*AP\*CP\*GP\*TP\*GP\*CP\*TP\*AP\*CP\*TP\*C)-3'

Chain H: 



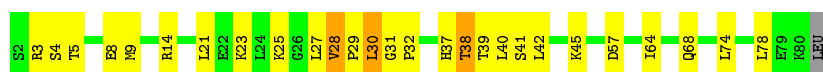
- Molecule 1: 5'-D(\*GP\*AP\*GP\*TP\*AP\*GP\*CP\*AP\*CP\*GP\*TP\*GP\*CP\*TP\*AP\*CP\*TP\*C)-3'

Chain J: 

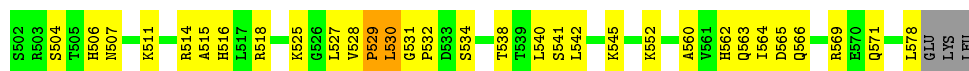


- Molecule 2: MAD PROTEIN

Chain A: 



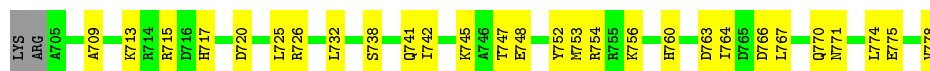
- Molecule 2: MAD PROTEIN



- Molecule 3: MAX PROTEIN



- Molecule 3: MAX PROTEIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.35Å 56.02Å 65.60Å 88.82° 79.08° 67.11°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.264 , 0.324	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4212	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	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	F	0.41	0/410	0.69	0/631
1	G	0.42	0/410	0.74	0/631
1	H	0.35	0/410	0.69	0/631
1	J	0.34	0/410	0.68	0/631
2	A	0.34	0/640	0.55	1/852 (0.1%)
2	D	0.34	0/615	0.51	0/821
3	B	0.46	0/646	0.52	0/862
3	E	0.35	0/626	0.49	0/837
All	All	0.38	0/4167	0.60	1/5896 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	32	PRO	N-CA-CB	5.69	110.13	103.30

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	F	366	0	204	19	0
1	G	366	0	204	13	0
1	H	366	0	204	12	0
1	J	366	0	204	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	634	0	652	39	0
2	D	609	0	633	40	0
3	B	637	0	632	36	0
3	E	617	0	606	32	0
4	A	36	0	0	1	0
4	B	38	0	0	5	0
4	D	41	0	0	3	0
4	E	28	0	0	1	0
4	F	26	0	0	0	0
4	G	38	0	0	0	0
4	H	23	0	0	0	0
4	J	21	0	0	0	0
All	All	4212	0	3339	176	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 24.

The worst 5 of 176 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:F:109:DA:H2"	1:F:110:DC:H5"	1.49	0.94
1:F:105:DT:H2"	1:F:106:DA:C8	2.06	0.90
2:D:566:GLN:HE22	2:D:569:ARG:HH21	1.21	0.88
2:D:578:LEU:HD21	3:E:778:VAL:HG22	1.56	0.86
2:D:527:LEU:HD22	3:E:754:ARG:HH22	1.42	0.84

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	
2	A	77/80 (96%)	69 (90%)	6 (8%)	2 (3%)	7	2
2	D	75/80 (94%)	71 (95%)	3 (4%)	1 (1%)	15	7
3	B	74/76 (97%)	72 (97%)	1 (1%)	1 (1%)	14	6
3	E	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
All	All	298/312 (96%)	282 (95%)	12 (4%)	4 (1%)	15	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	231	SER
2	A	30	LEU
2	A	28	VAL
2	D	529	PRO

### 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	
2	A	67/75 (89%)	66 (98%)	1 (2%)	72	75
2	D	66/75 (88%)	65 (98%)	1 (2%)	72	75
3	B	68/69 (99%)	65 (96%)	3 (4%)	35	30
3	E	66/69 (96%)	64 (97%)	2 (3%)	48	47
All	All	267/288 (93%)	260 (97%)	7 (3%)	54	54

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	269	ARG
3	E	766	ASP
2	D	530	LEU
3	B	216	ASP
3	E	725	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such

sidechains are listed below:

Mol	Chain	Res	Type
2	D	506	HIS
2	D	562	HIS
3	E	707	HIS
3	B	258	HIS
3	E	706	HIS

### 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 will therefore be empty.

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

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

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