



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:39 PM GMT

PDB ID : 1GLU  
Title : CRYSTALLOGRAPHIC ANALYSIS OF THE INTERACTION OF THE  
GLUCOCORTICOID RECEPTOR WITH DNA  
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Sigler, P.B.  
Deposited on : 1992-08-30  
Resolution : 2.90 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

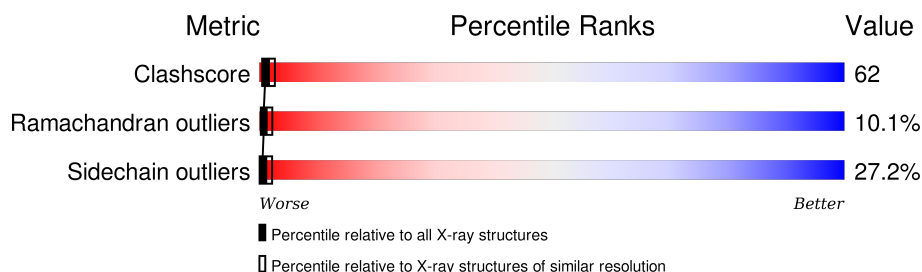
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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	19	
1	D	19	
2	A	81	
2	B	81	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2071 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 DNA (5'-D(\*CP\*CP\*AP\*GP\*AP\*AP\*CP\*AP\*TP\*CP\*GP\*AP\*TP\*GP\*TP\*TP\*C P\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	19	Total	C	N	O	P	0	0	0
			385	185	70	112	18			
1	D	19	Total	C	N	O	P	0	0	0
			385	185	70	112	18			

- Molecule 2 is a protein called PROTEIN (GLUCOCORTICOID RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	81	Total	C	N	O	S	0	0	0
			628	385	124	107	12			
2	B	81	Total	C	N	O	S	0	0	0
			628	385	124	107	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	437	ALA	PRO	CONFLICT	UNP P06536
A	438	ARG	LYS	CONFLICT	UNP P06536
A	439	PRO	LEU	CONFLICT	UNP P06536
B	437	ALA	PRO	CONFLICT	UNP P06536
B	438	ARG	LYS	CONFLICT	UNP P06536
B	439	PRO	LEU	CONFLICT	UNP P06536

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	O 7	0	0
4	B	18	Total 18	O 18	0	0
4	C	7	Total 7	O 7	0	0
4	D	9	Total 9	O 9	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 ( $\text{RSRZ} > 2$ ). 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: DNA (5'-D(\*CP\*CP\*AP\*GP\*AP\*AP\*CP\*AP\*TP\*CP\*GP\*AP\*TP\*GP\*TP\*TP\*C P\*TP\*G)-3')

Chain C: 



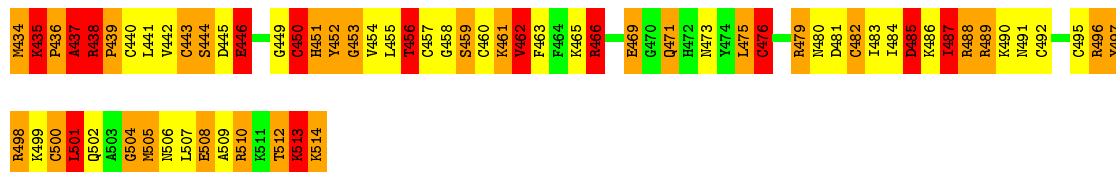
- Molecule 1: DNA (5'-D(\*CP\*CP\*AP\*GP\*AP\*AP\*CP\*AP\*TP\*CP\*GP\*AP\*TP\*GP\*TP\*TP\*C P\*TP\*G)-3')

Chain D: 



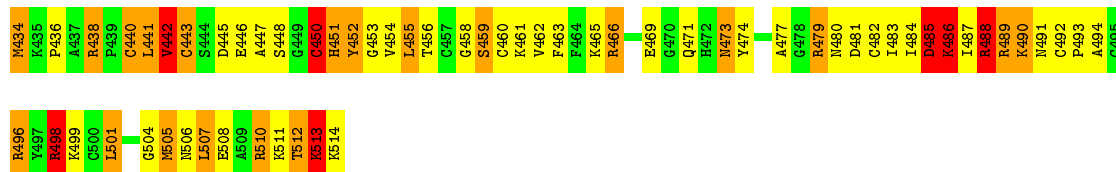
- Molecule 2: PROTEIN (GLUCOCORTICOID RECEPTOR)

Chain A: 



- Molecule 2: PROTEIN (GLUCOCORTICOID RECEPTOR)

Chain B: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.50Å 95.70Å 120.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR, PROLSQ	Depositor
R, $R_{free}$	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2071	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	2.49	23/431 (5.3%)	4.15	124/663 (18.7%)
1	D	2.62	27/431 (6.3%)	4.34	134/663 (20.2%)
2	A	1.01	0/637	2.11	32/848 (3.8%)
2	B	0.99	0/637	2.11	33/848 (3.9%)
All	All	1.80	50/2136 (2.3%)	3.23	323/3022 (10.7%)

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
1	D	0	2
2	A	0	10
2	B	0	6
All	All	0	20

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	-9	DC	P-O5'	-14.53	1.45	1.59
1	D	-7	DG	O3'-P	8.93	1.71	1.61
1	C	-7	DG	C4'-O4'	-8.78	1.36	1.45
1	D	-5	DA	O3'-P	8.03	1.70	1.61
1	C	6	DT	P-O5'	7.92	1.67	1.59

The worst 5 of 323 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-10	DC	P-O3'-C3'	21.88	145.96	119.70
1	D	-5	DA	O4'-C1'-N9	19.24	121.47	108.00
1	C	-3	DA	O4'-C1'-N9	17.65	120.36	108.00
1	C	4	DG	O5'-P-OP2	17.35	131.52	110.70
1	D	-10	DC	O4'-C1'-N1	17.34	120.14	108.00

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	435	LYS	Mainchain
1	C	-3	DA	Sidechain
1	C	3	DT	Sidechain
1	D	-8	DA	Sidechain
1	D	6	DT	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	385	0	216	28	0
1	D	385	0	216	32	0
2	A	628	0	635	116	0
2	B	628	0	637	73	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	7	0	0	2	0
4	B	18	0	0	4	0
4	C	7	0	0	1	0
4	D	9	0	0	3	0
All	All	2071	0	1704	228	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 62.

The worst 5 of 228 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:A:450:CYS:SG	2:A:513:LYS:HG2	1.70	1.29
2:A:437:ALA:O	2:A:439:PRO:HD2	1.15	1.29
2:A:437:ALA:O	2:A:439:PRO:CD	1.85	1.25
2:A:475:LEU:HD23	2:B:488:ARG:NH1	1.61	1.15
2:A:446:GLU:O	2:A:446:GLU:HG2	1.42	1.14

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	
2	A	79/81 (98%)	51 (65%)	18 (23%)	10 (13%)	0	1
2	B	79/81 (98%)	58 (73%)	15 (19%)	6 (8%)	1	3
All	All	158/162 (98%)	109 (69%)	33 (21%)	16 (10%)	1	2

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	436	PRO
2	A	437	ALA
2	A	438	ARG
2	A	452	TYR
2	A	500	CYS

### 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	
2	A	68/68 (100%)	47 (69%)	21 (31%)	0	1
2	B	68/68 (100%)	52 (76%)	16 (24%)	1	2
All	All	136/136 (100%)	99 (73%)	37 (27%)	0	2

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	501	LEU
2	A	514	LYS
2	B	507	LEU
2	A	508	GLU
2	A	510	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	473	ASN
2	A	491	ASN
2	B	451	HIS
2	B	473	ASN
2	B	506	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.