



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 03:01 PM GMT

PDB ID : 1R4R
Title : Crystallographic analysis of the interaction of the glucocorticoid receptor with DNA
Authors : Luisi, B.F.; Xu, W.X.; Otwinowski, Z.; Freedman, L.P.; Yamamoto, K.R.; Sigler, P.B.
Deposited on : 2003-10-07
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

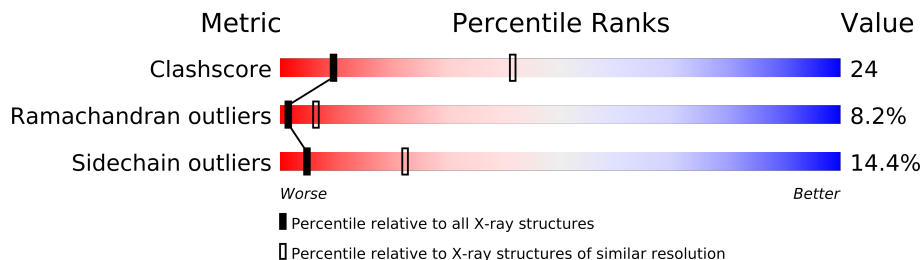
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	19	
2	D	19	
3	A	92	
3	B	92	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2314 atoms, of which 380 are hydrogens and 0 are deuterium.

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(*TP*CP*AP*GP*AP*AP*CP*AP*TP*GP*AP*T
P*GP*TP*TP*CP*TP*CP*A)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	19	Total	C	H	N	O	P	0	0	0
			422	186	37	69	112	18			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	19	Total	C	H	N	O	P	0	0	0
			424	186	38	69	113	18			

- Molecule 3 is a protein called Glucocorticoid receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	73	Total	C	H	N	O	S	0	0	0
			714	344	149	112	98	11			
3	B	77	Total	C	H	N	O	S	0	0	0
			750	363	156	117	102	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	434	MET	-	CLONING ARTIFACT	UNP P06536
A	435	LYS	-	CLONING ARTIFACT	UNP P06536
A	436	PRO	-	CLONING ARTIFACT	UNP P06536
A	437	ALA	-	CLONING ARTIFACT	UNP P06536
A	438	ARG	-	CLONING ARTIFACT	UNP P06536
A	439	PRO	-	CLONING ARTIFACT	UNP P06536
B	434	MET	-	CLONING ARTIFACT	UNP P06536
B	435	LYS	-	CLONING ARTIFACT	UNP P06536
B	436	PRO	-	CLONING ARTIFACT	UNP P06536
B	437	ALA	-	CLONING ARTIFACT	UNP P06536

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Chain	Residue	Modelled	Actual	Comment	Reference
B	438	ARG	-	CLONING ARTIFACT	UNP P06536
B	439	PRO	-	CLONING ARTIFACT	UNP P06536

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Zn 2	0	0
4	A	2	Total 2	Zn 2	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(*TP*CP*AP*GP*AP*AP*CP*AP*TP*GP*AP*TP*GP*TP*TP*CP*TP*CP*A)-3'

Chain C: 



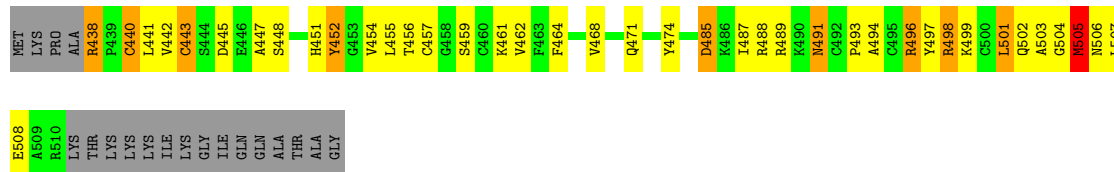
- Molecule 2: 5'-D(*CP*TP*GP*AP*GP*AP*AP*CP*AP*TP*CP*AP*TP*GP*TP*TP*CP*TP*G)-3'

Chain D: 



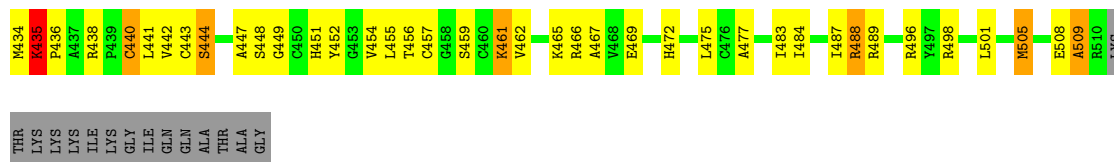
- Molecule 3: Glucocorticoid receptor

Chain A: 



- Molecule 3: 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, α , β , γ	38.50Å 99.70Å 121.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2314	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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	2.48	21/431 (4.9%)	3.56	86/663 (13.0%)
2	D	2.29	16/432 (3.7%)	3.36	74/665 (11.1%)
3	A	0.39	0/573	0.70	0/765
3	B	0.40	0/603	0.63	0/805
All	All	1.58	37/2039 (1.8%)	2.39	160/2898 (5.5%)

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	4
2	D	0	4
All	All	0	8

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	DC	P-O5'	10.92	1.70	1.59
1	C	12	DT	C5-C7	10.24	1.56	1.50
1	C	15	DT	C5-C7	9.22	1.55	1.50
1	C	3	DA	N9-C4	-8.66	1.32	1.37
1	C	12	DT	P-O5'	-7.91	1.51	1.59

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	19	DG	C1'-O4'-C4'	-19.83	90.27	110.10
2	D	13	DT	O4'-C1'-N1	15.95	119.16	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	DA	C1'-O4'-C4'	-15.92	94.18	110.10
2	D	5	DG	C1'-O4'-C4'	-15.04	95.06	110.10
1	C	16	DC	O4'-C1'-C2'	-15.03	93.88	105.90

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	10	DG	Sidechain
1	C	11	DA	Sidechain
1	C	17	DT	Sidechain
1	C	8	DA	Sidechain
2	D	2	DT	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	385	37	180	7	0
2	D	386	38	179	9	0
3	A	565	149	408	37	0
3	B	594	156	436	38	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
All	All	1934	380	1203	84	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

The worst 5 of 84 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:487:ILE:HD13	3:B:475:LEU:HD12	1.56	0.88
3:B:498:ARG:HB3	3:B:498:ARG:HH11	1.44	0.82
1:C:13:DG:H5'	3:B:489:ARG:HH21	1.47	0.79
3:A:468:VAL:HG11	3:A:507:LEU:HD22	1.65	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:489:ARG:HD2	3:A:496:ARG:HH12	1.54	0.71

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	71/92 (77%)	51 (72%)	15 (21%)	5 (7%)	2	9
3	B	75/92 (82%)	51 (68%)	17 (23%)	7 (9%)	1	5
All	All	146/184 (79%)	102 (70%)	32 (22%)	12 (8%)	1	6

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	491	ASN
3	B	444	SER
3	A	505	MET
3	B	435	LYS
3	B	449	GLY

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	61/75 (81%)	50 (82%)	11 (18%)	2	13
3	B	64/75 (85%)	57 (89%)	7 (11%)	9	35
All	All	125/150 (83%)	107 (86%)	18 (14%)	5	22

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	501	LEU
3	A	502	GLN
3	B	469	GLU
3	A	496	ARG
3	A	498	ARG

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

Mol	Chain	Res	Type
3	A	480	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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.

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 ⓘ

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.